

10541328

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10541328

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 10:41:20 ON 04 AUG 2008

```
=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
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Choice (Y/n):
```

Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:41:35 ON 04 AUG 2008
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 AUG 2008 HIGHEST RN 1037774-47-2

SCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

DECODED: A detailed description of the search algorithm and its performance is provided in the accompanying paper.

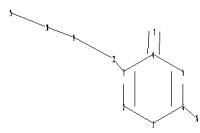
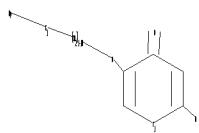
10541328

experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10541328.str



chain nodes :
7 9 10 12 15 16
ring nodes :
1 2 3 4 5 6
chain bonds :
3-12 4-7 6-16 9-10 9-12 10-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 3-12 4-5 4-7 5-6 6-16 9-10 9-12 10-15
isolated ring systems :
containing 1 :

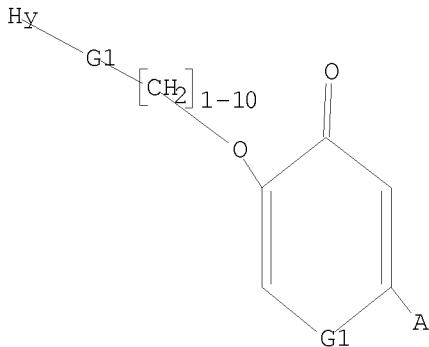
G1:O,S,N

10541328

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:Atom 12:CLASS
15:Atom 16:CLASS

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR



G1 O, S, N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 10:41:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 27269 TO ITERATE

7.3% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 535500 TO 555260
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 sss full
FULL SEARCH INITIATED 10:41:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 553581 TO ITERATE

100.0% PROCESSED 553581 ITERATIONS 69 ANSWERS
SEARCH TIME: 00.00.08

L3 69 SEA SSS FUL L1

10541328

=> FIL HCAPLUS	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	178.36	178.57

FILE 'HCAPLUS' ENTERED AT 10:42:11 ON 04 AUG 2008
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FILE COVERS 1907 - 4 Aug 2008 VOL 149 ISS 6
FILE LAST UPDATED: 3 Aug 2008 (20080803/ED)

HCAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 5 L3

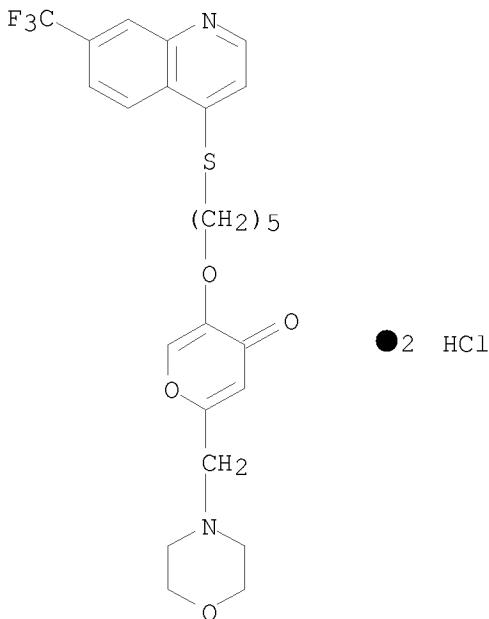
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L5 1 L4 AND PY<=2003

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L4 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:622524 HCAPLUS
TITLE: Characterization of EHT 1864, a novel small molecule inhibitor of Rac family small GTPases
AUTHOR(S): Onesto, Cercina; Shutes, Adam; Picard, Virginie; Schweighoffer, Fabien; Der, Channing J.
CORPORATE SOURCE: Lineberger Comprehensive Cancer Center, Department of Pharmacology, University of North Carolina at Chapel Hill, Chapel Hill, NC, USA
SOURCE: Methods in Enzymology (2008), 439 (Small GTPases in Disease, Part B), 111-129
CODEN: MENZAU; ISSN: 0076-6879
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. There is now considerable exptl. evidence that aberrant

activation of Rho family small GTPases promotes uncontrolled proliferation, invasion, and metastatic properties of human cancer cells. Therefore, there is considerable interest in the development of small mol. inhibitors of Rho GTPase function. However, to date, most efforts have focused on inhibitors that block Rho GTPase function indirectly, either by targeting enzymes involved in post-translational processing or downstream protein kinase effectors. We have reported the identification and characterization of the EHT 1864 small mol. as an inhibitor of Rac family small GTPases, placing Rac1 in an inert and inactive state and then impairing Rac1-mediated functions in vivo. Our work suggests that EHT 1864 selectively inhibits Rac1 downstream signaling and cellular transformation by a novel mechanism involving guanine nucleotide displacement. This chapter provides the details for some of the biochem. and biol. methods used to characterize the mode of action of EHT 1864 on Rac1 and its impact on Rac1-dependent cellular functions.

IT 754240-09-0, EHT1864
 RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (biochem. and biol. methods may be useful to characterize Rho GTPase specificity and mechanism of action of EHT 1864 on Rac1 and its impact on Rac1-dependent cellular function in mouse)
 RN 754240-09-0 HCPLUS
 CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-, hydrochloride (1:2) (CA INDEX NAME)



L4 ANSWER 2 OF 5 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:1368320 HCPLUS
 DOCUMENT NUMBER: 148:232138
 TITLE: Specificity and Mechanism of Action of EHT 1864, a Novel Small Molecule Inhibitor of Rac Family Small GTPases

AUTHOR(S): Shutes, Adam; Onesto, Cercina; Picard, Virginie; Leblond, Bertrand; Schweighoffer, Fabien; Der, Channing J.

CORPORATE SOURCE: Lineberger Comprehensive Cancer Center, University of North Carolina, Chapel Hill, NC, 27599, USA

SOURCE: Journal of Biological Chemistry (2007), 282(49), 35666-35678

CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

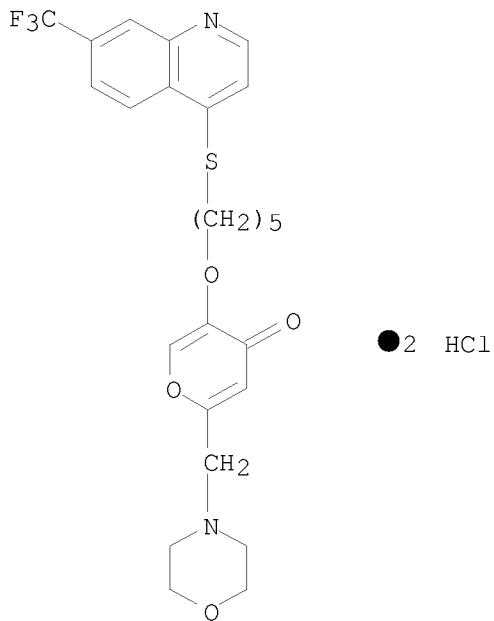
AB There is now considerable exptl. evidence that aberrant activation of Rho family small GTPases promotes the uncontrolled proliferation, invasion, and metastatic properties of human cancer cells. Therefore, there is considerable interest in the development of small mol. inhibitors of Rho GTPase function. However, to date, most efforts have focused on inhibitors that indirectly block Rho GTPase function, by targeting either enzymes involved in post-translational processing or downstream protein kinase effectors. We recently determined that the EHT 1864 small mol. can inhibit Rac function in vivo. In this study, we evaluated the biol. and biochem. specificities and biochem. mechanism of action of EHT 1864. We determined that EHT 1864 specifically inhibited Rac1-dependent platelet-derived growth factor-induced lamellipodia formation. Furthermore, our biochem. analyses with recombinant Rac proteins found that EHT 1864 possesses high affinity binding to Rac1, as well as the related Rac1b, Rac2, and Rac3 isoforms, and this association promoted the loss of bound nucleotide, inhibiting both guanine nucleotide association and Tiam1 Rac guanine nucleotide exchange factor-stimulated exchange factor activity in vitro. EHT 1864 therefore places Rac in an inert and inactive state, preventing its engagement with downstream effectors. Finally, we evaluated the ability of EHT 1864 to block Rac-dependent growth transformation, and we determined that EHT 1864 potently blocked transformation caused by constitutively activated Rac1, as well as Rac-dependent transformation caused by Tiam1 or Ras. Taken together, our results suggest that EHT 1864 selectively inhibits Rac downstream signaling and transformation by a novel mechanism involving guanine nucleotide displacement.

IT 754240-09-0, EHT 1864

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(EHT 1864 specifically inhibits Rac1-dependent platelet-derived growth factor-induced lamellipodia formation)

RN 754240-09-0 HCAPLUS

CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]-, hydrochloride (1:2) (CA INDEX NAME)



REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 5 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1191062 HCPLUS
DOCUMENT NUMBER: 144:68139
TITLE: RAC1 Inhibition Targets Amyloid Precursor Protein Processing by γ -Secretase and Decreases A β Production in Vitro and in Vivo
AUTHOR(S): Desire, Laurent; Bourdin, Jerome; Loiseau, Nadia; Peillon, Helene; Picard, Virginie; De Oliveira, Catherine; Bachelot, Florence; Leblond, Bertrand; Taverne, Thierry; Beausoleil, Eric; Lacombe, Sandrine; Drouin, Dominique; Schweighoffer, Fabien
CORPORATE SOURCE: Exonhit Therapeutics, Paris, 75013, Fr.
SOURCE: Journal of Biological Chemistry (2005), 280(45), 37516-37525
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB β -Amyloid peptides (A β) that form the senile plaques of Alzheimer disease consist mainly of 40- and 42-amino acid (A β 40 and A β 42) peptides generated from the cleavage of the amyloid precursor protein (APP). Generation of A β involves β -secretase and γ -secretase activities and is regulated by membrane trafficking of the proteins involved in A β production. Here we describe a new small mol., EHT 1864, which blocks the Rac1 signaling pathways. In vitro, EHT 1864 blocks A β 40 and A β 42 production but does not impact SAPP α levels and does not inhibit β -secretase. Rather, EHT 1864 modulates APP processing at the level of γ -secretase to prevent

A β 40 and A β 42 generation. This effect does not result from a direct inhibition of the γ -secretase activity and is specific for APP cleavage, since EHT 1864 does not affect Notch cleavage. In vivo, EHT 1864 significantly reduces A β 40 and A β 42 levels in guinea pig brains at a threshold that is compatible with delaying plaque accumulation and/or clearing the existing plaque in brain. EHT 1864 is the first derivative of a new chemical series that consists of candidates for inhibiting A β formation in the brain of AD patients. Our findings represent the first pharmacol. validation of Rac1 signaling as a target for developing novel therapies for Alzheimer disease.

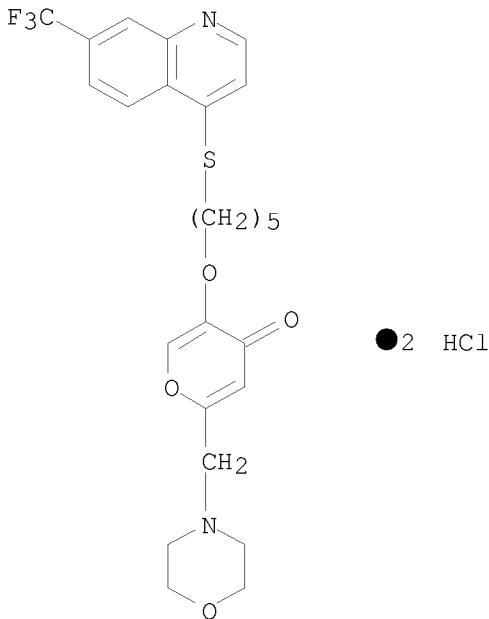
IT 754240-09-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(EHT 1864; EHT 1864 blocked A β 1-40 and A β 1-42 production)

RN 754240-09-0 HCPLUS

CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]-, hydrochloride (1:2) (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 5 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:740320 HCPLUS

DOCUMENT NUMBER: 141:260557

TITLE: Preparation of novel antiproliferative and antiangiogenic agents, in particular

quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis

Leblond, Bertrand; Petit, Silvere; Picard, Virginie;

Taverne, Thierry; Schweighoffer, Fabien

INVENTOR(S):

PATENT ASSIGNEE(S): Exonhit Therapeutics Sa, Fr.

SOURCE: PCT Int. Appl., 156 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

1

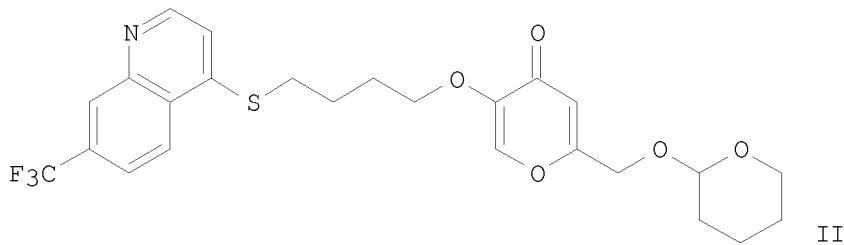
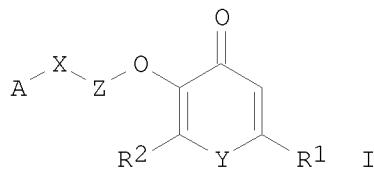
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004076445	A2	20040910	WO 2004-IB926	20040227
WO 2004076445	A3	20050106		
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EP 1471063	A1	20041027	EP 2003-290490	20030228
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AU 2004215577	A1	20040910	AU 2004-215577	20040227
CA 2516239	A1	20040910	CA 2004-2516239	20040227
EP 1597253	A2	20051123	EP 2004-715422	20040227
EP 1597253	B1	20060809		
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CN 1747952	A	20060315	CN 2004-80003820	20040227
JP 2006519221	T	20060824	JP 2006-502497	20040227
AT 335734	T	20060915	AT 2004-715422	20040227
US 20060183749	A1	20060817	US 2005-541328	20050830
PRIORITY APPLN. INFO.:			EP 2003-290490	A 20030228
			WO 2004-IB926	W 20040227

OTHER SOURCE(S):

MARPAT 141:260557

GI



AB Title compds. I [wherein R1 = [(tetrahydropyran-2-yl)oxygen]methyl, CH2-B, (morpholin-4-yl)methyl, pyrrolidin-1-ylmethyl, etc.; B = halo, OH, OCH2OMe, OCH2OCH2CH2OMe, OSO2-alkyl, OTBDMS; R2 = H, alk(en)yl; X, Y = independently O, S, NH and derivs.; A = quinolin-4-yl, quinolin-8-yl, benzo[b]thiophen-7-yl, quinazolin-4-yl; Z = (CH2)n, optionally interrupted by a heteroatom, C(:O) or aryldialkyl, especially xlenyl, group; n = 1-10; their tautomers, optical and geometrical isomers, racemates, salts, hydrates and mixts.] were prepared as antiproliferative agents and angiogenesis inhibitors. Nine biol. assays are given. For example, II was prepared, in 2 steps, from pyranone III, 1,4-dibromobutane, and 7-(trifluoromethyl)-4-quinolinethiol. In an in vitro cell viability assay, selected I showed an IC50 < 4 μ M and < 9 μ M against HCT116 and MDA-MB-231 tumoral cell lines, demonstrating their cytostatic mode of action. I are useful for treating various diseases associated with abnormal cell proliferation, including cancer, especially leukemia, or associated with unregulated angiogenesis including growth and metastasis of solid tumors, ocular diseases, especially retinopathies, or arthritis.

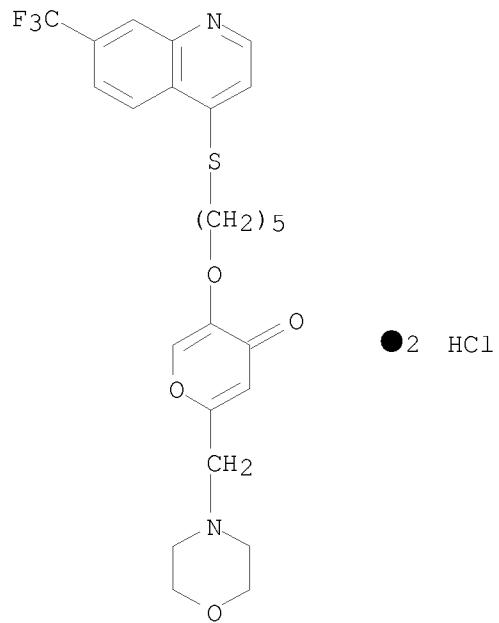
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 754240-17-0P, 5-[(5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl)oxy]-2-[(4-methylpiperazin-1-yl)methyl]-4H-pyran-4-one trihydrochloride 754240-19-2P, 5-[(5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl)oxy]-2-[(piperazin-1-yl)methyl]-4H-pyran-4-one trihydrochloride

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)

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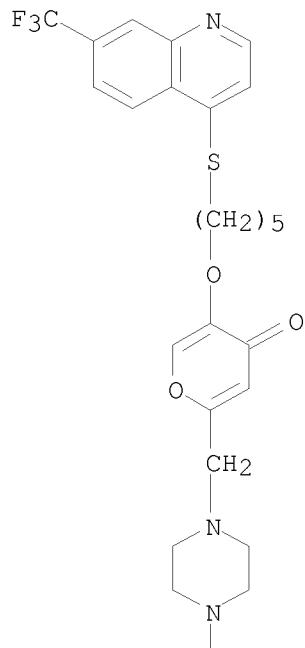
quinolinyl]thio]pentyl]oxy]-, hydrochloride (1:2) (CA INDEX NAME)



RN 754240-17-0 HCPLUS

CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[[5-[(7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-, hydrochloride (1:3) (CA INDEX NAME)

PAGE 1-A

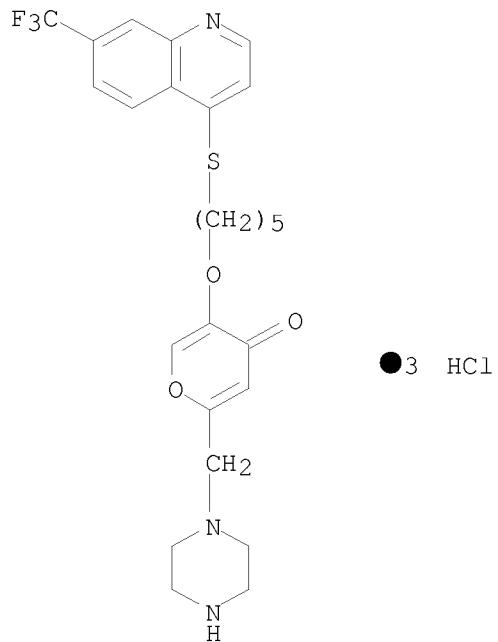


PAGE 2-A



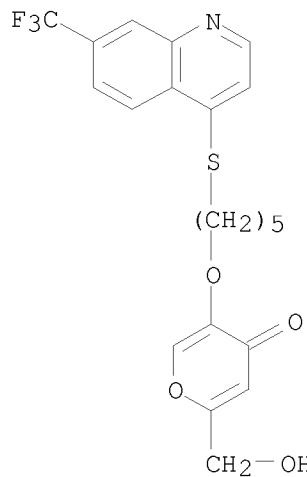
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RN 754240-19-2 HCPLUS
CN 4H-Pyran-4-one, 2-(1-piperazinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thiopentyl]oxy]-, hydrochloride (1:3) (CA INDEX NAME)



IT 754239-59-3P, 2-Hydroxymethyl-5-[[5-[7-(trifluoromethyl)quinolin-4-ylsulfanyl]pentyl]oxy]-4H-pyran-4-one 754240-15-8P, tert-Butyl 4-[[5-[[5-[7-(trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]piperazine-1-carboxylate 754240-16-9P, tert-Butyl 4-[[5-[[5-(7-chloroquinolin-4-yloxy)pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]piperazine-1-carboxylate
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate; preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)

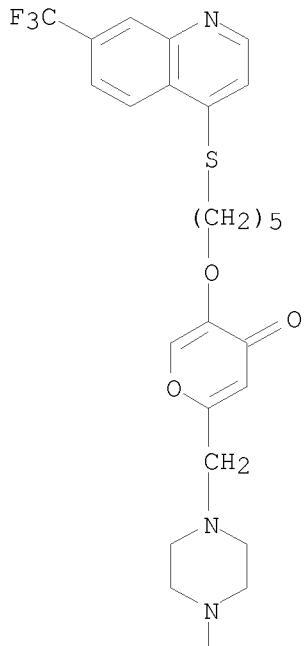
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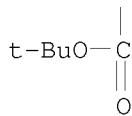
RN 754240-15-8 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[4-oxo-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-4H-pyran-2-yl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

PAGE 1-A



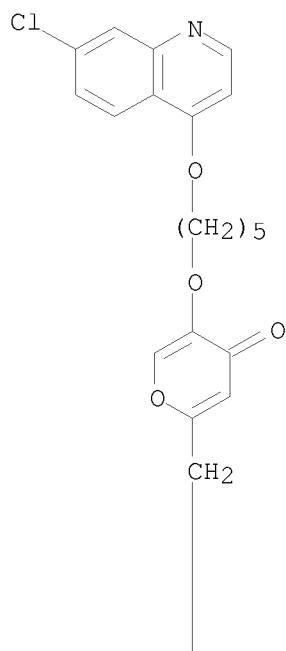
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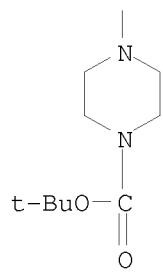
RN 754240-16-9 HCPLUS

CN 1-Piperazinecarboxylic acid, 4-[[5-[[5-[(7-chloro-4-quinolinyloxy]pentyloxy]-4-oxo-4H-pyran-2-yl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



IT 754239-47-9P, 5-[[5-(6-Fluoro-2-methylquinolin-4-yloxy)pentyl]oxy]-2-[(tetrahydropyran-2-yl)oxy]methyl]-4H-pyran-4-one 754239-48-0P

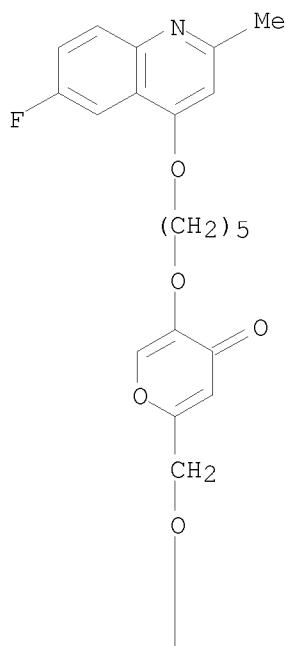
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 4H-pyran-4-one hydrochloride 754239-60-6P, 2-
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 (trifluoromethyl)quinolin-4-yl]sulfanyl]pentyl]oxy]-4H-pyran-4-one
 754239-66-2P, 5-[[7-[7-(Trifluoromethyl)quinolin-4-
 ylthio]heptyl]oxy]-2-[[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-4H-pyran-4-
 one 754239-68-4P, 5-[[8-[7-(Trifluoromethyl)quinolin-4-
 ylthio]octyl]oxy]-2-[[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-4H-pyran-4-one
 754239-80-0P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-
 ylthio]pentyl]oxy]-2-[(piperidin-1-yl)methyl]-4H-pyran-4-one
 754239-81-1P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-
 ylthio]pentyl]oxy]-2-(thiomorpholinomethyl)-4H-pyran-4-one
 754239-82-2P, 2-[(Diethylamino)methyl]-5-[[5-[7-
 (trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4H-pyran-4-one
 754239-83-3P, 5-[[5-[6-(Trifluoromethyl)quinolin-4-
 yloxy]pentyl]oxy]-2-(morpholinomethyl)-4H-pyran-4-one 754239-84-4P
 , 5-[[5-[7-(Trifluoromethyl)quinolin-4-yloxy]pentyl]oxy]-2-[(4-
 methylpiperazin-1-yl)methyl]-4H-pyran-4-one 754239-85-5P,
 5-[[5-[7-(Trifluoromethyl)quinolin-4-yloxy]pentyl]oxy]-2-
 (morpholinomethyl)-4H-pyran-4-one 754239-86-6P,
 4-[[5-[[6-(4-Methylpiperazin-1-ylmethyl)-4-oxo-4H-pyran-3-
 yl]oxy]pentyl]oxy]-7-trifluoromethylquinoline-3-carboxylic acid ethyl
 ester 754239-87-7P, 4-[[5-[[6-(Morpholin-4-yl)methyl]-4-oxo-4H-
 pyran-3-yl]oxy]pentyl]oxy]-7-trifluoromethylquinoline-3-carboxylic acid
 ethyl ester 754239-88-8P, 5-[[5-[8-(Trifluoromethyl)quinolin-4-
 yloxy]pentyl]oxy]-2-[(4-methylpiperazin-1-yl)methyl]-4H-pyran-4-one
 754239-89-9P, 5-[[5-[8-(Trifluoromethyl)quinolin-4-
 yloxy]pentyl]oxy]-2-(morpholinomethyl)-4H-pyran-4-one 754239-90-2P
 , 5-[[5-(Quinazolin-4-yloxy)pentyl]oxy]-2-[(pyrrolidin-1-yl)methyl]-4H-
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 2-(morpholinomethyl)-4H-pyran-4-one 754239-92-4P,
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 4H-pyran-4-one 754239-93-5P, 5-[[5-[7-(Trifluoromethyl)quinolin-
 4-ylthio]pentyl]oxy]-2-(fluoromethyl)-4H-pyran-4-one 754240-07-8P
 , 5-[2-[7-(Trifluoromethyl)quinolin-4-ylthio]ethoxy]-2-[[[(tetrahydro-2H-
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 trihydrochloride 754240-21-6P, 5-[[5-[7-

(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-[(4-acetylpirazin-1-yl)methyl]-4H-pyran-4-one 754240-22-7P, 4-[[5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]-N,N-diethylpirazin-1-carboxamide 754240-23-8P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-[(4-(pivaloyl)piperazin-1-yl)methyl]-4H-pyran-4-one 754240-24-9P, 4-[[5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]-N,N-diisopropylpirazin-1-carboxamide 754240-25-0P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-[(4-Methylsulfonylpiperazin-1-yl)methyl]-4H-pyran-4-one 754240-26-1P, 4-[[5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]-N-tert-butylpiperazin-1-carboxamide 754240-27-2P, 4-[[5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]-N-methylpirazin-1-carboxamide 754240-28-3P, 5-[[5-(7-Chloroquinolin-4-yl)oxy]pentyl]oxy]-2-[(piperazin-1-yl)methyl]-4H-pyran-4-one
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)

RN 754239-47-9 HCPLUS

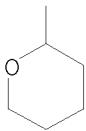
CN 4H-Pyran-4-one, 5-[[5-[(6-fluoro-2-methyl-4-quinolinyl)oxy]pentyl]oxy]-2-[(tetrahydro-2H-pyran-2-yl)oxy]methyl- (CA INDEX NAME)

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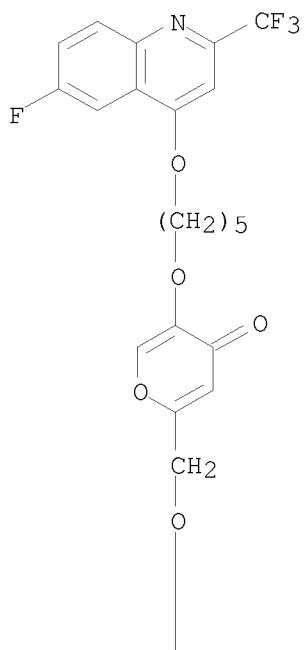
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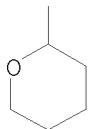


RN 754239-48-0 HCAPLUS
CN 4H-Pyran-4-one, 5-[5-[6-fluoro-2-(trifluoromethyl)-4-quinolinyl]oxy]pentyl]oxy]-2-[(tetrahydro-2H-pyran-2-yl)oxy]methyl]- (CA INDEX NAME)

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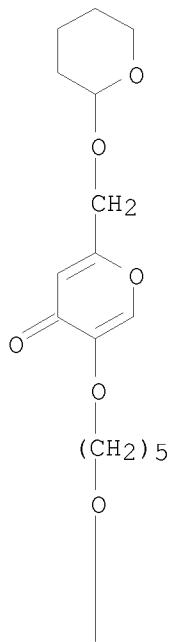
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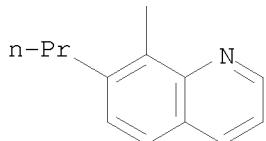
RN 754239-49-1 HCAPLUS
CN 4H-Pyran-4-one, 5-[5-[(7-propyl-8-quinolinyl)oxy]pentyl]oxy]-2-[(tetrahydro-2H-pyran-2-yl)oxy]methyl]- (CA INDEX NAME)

10541328

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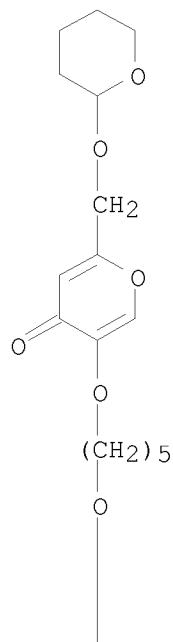


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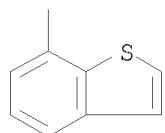


RN 754239-50-4 HCPLUS
CN 4H-Pyran-4-one, 5-[[5-(benzo[b]thien-7-yl)oxy]pentyl]oxy]-2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]- (CA INDEX NAME)

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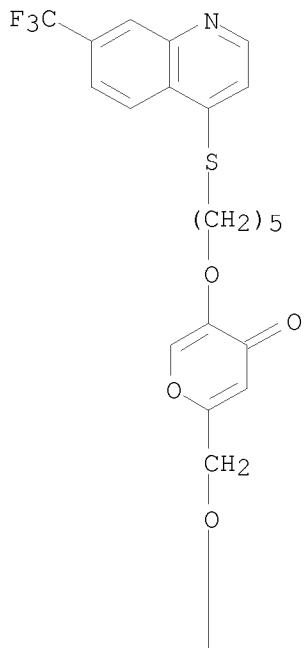


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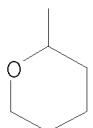


RN 754239-51-5 HCPLUS
CN 4H-Pyran-4-one, 2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thiopentyl]oxy]- (CA INDEX NAME)

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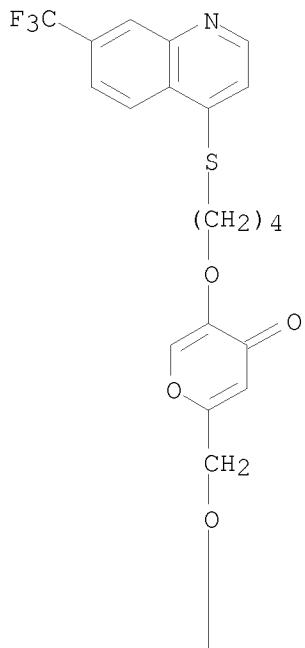
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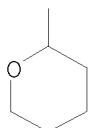
RN 754239-53-7 HCPLUS

CN 4H-Pyran-4-one, 2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[4-[[7-(trifluoromethyl)-4-quinolinyl]thio]butoxy]- (CA INDEX NAME)

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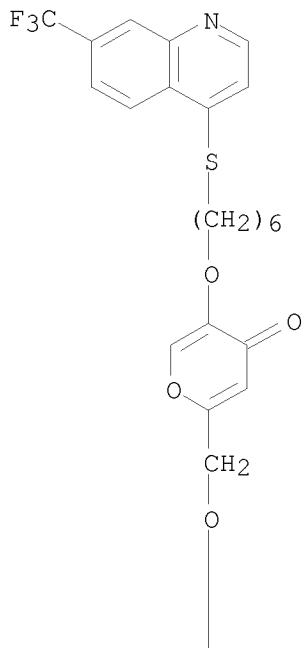
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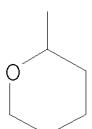
RN 754239-55-9 HCPLUS

CN 4H-Pyran-4-one, 2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[[6-[[7-(trifluoromethyl)-4-quinolinyl]thio]hexyl]oxy]- (CA INDEX NAME)

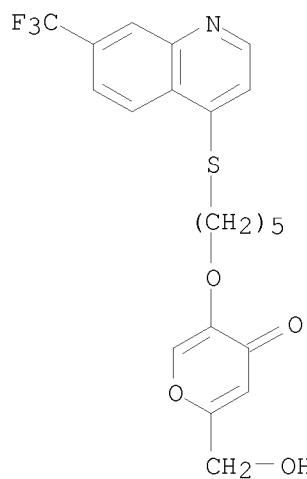
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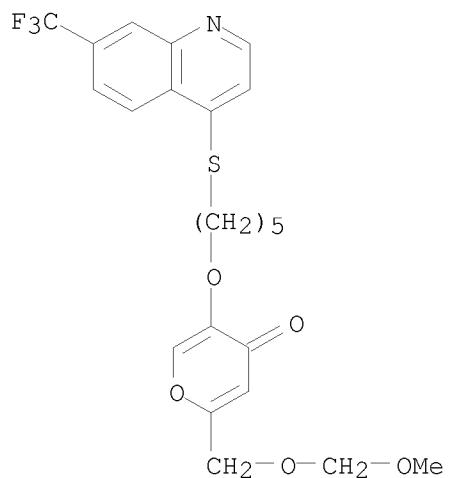
RN 754239-56-0 HCPLUS
CN 4H-Pyran-4-one, 2-(hydroxymethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

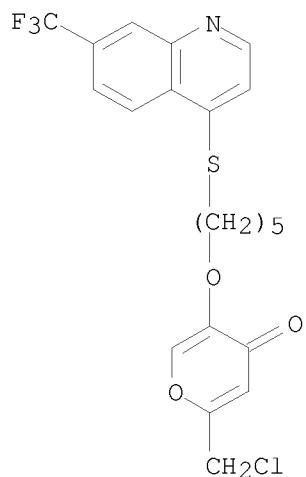
RN 754239-60-6 HCPLUS

CN 4H-Pyran-4-one, 2-[(methoxymethoxy)methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



RN 754239-62-8 HCPLUS

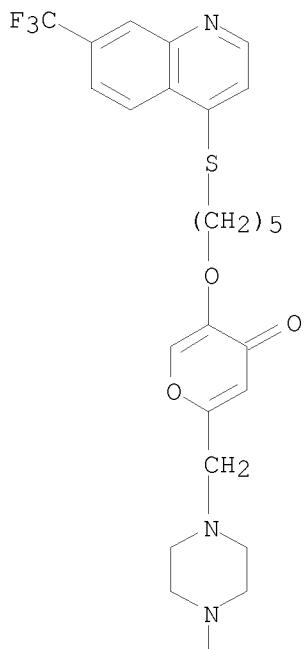
CN 4H-Pyran-4-one, 2-(chloromethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



RN 754239-63-9 HCPLUS

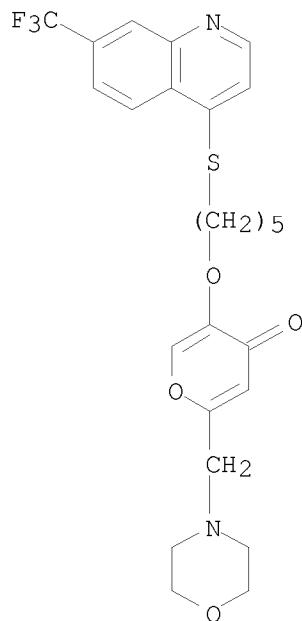
CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[[5-[(7-(trifluoromethyl)-4-quinolinyloxy)pentyl]thio]pentyl]oxy]- (CA INDEX NAME)

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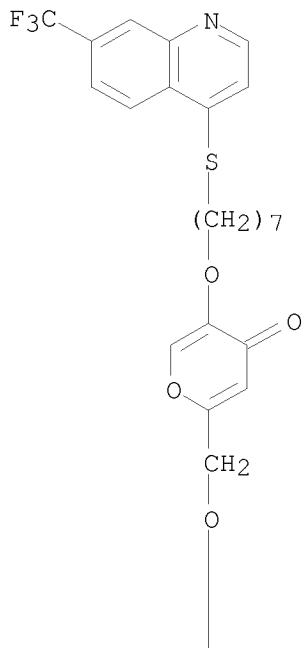
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Me

RN 754239-64-0 HCAPLUS
CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]- (CA INDEX NAME)

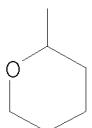


RN 754239-66-2 HCAPLUS
CN 4H-Pyran-4-one, 2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[[7-[[7-(trifluoromethyl)-4-quinolinyl]thio]heptyloxy]- (CA INDEX NAME)

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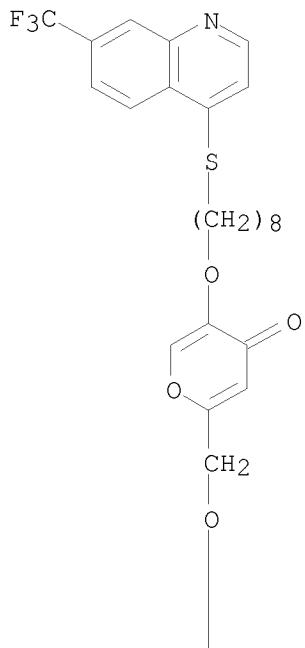


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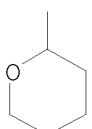


RN 754239-68-4 HCPLUS
CN 4H-Pyran-4-one, 2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[[8-[[7-(trifluoromethyl)-4-quinolinyl]thio]octyl]oxy]- (CA INDEX NAME)

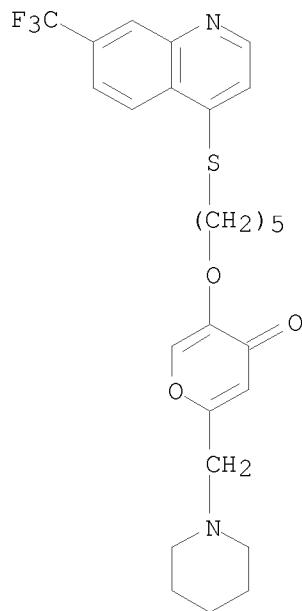
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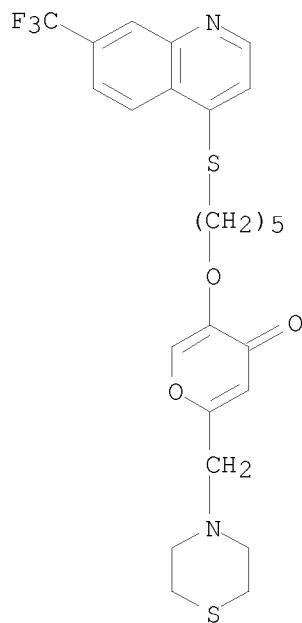


RN 754239-80-0 HCPLUS
CN 4H-Pyran-4-one, 2-(1-piperidinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



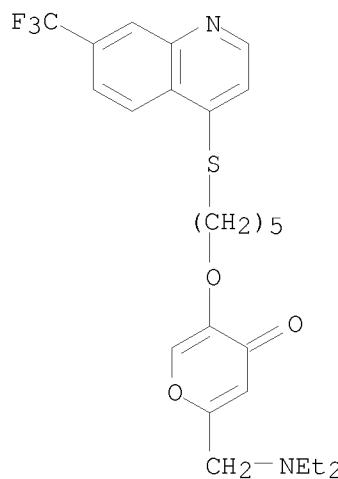
RN 754239-81-1 HCAPLUS

CN 4H-Pyran-4-one, 2-(4-thiomorpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]- (CA INDEX NAME)



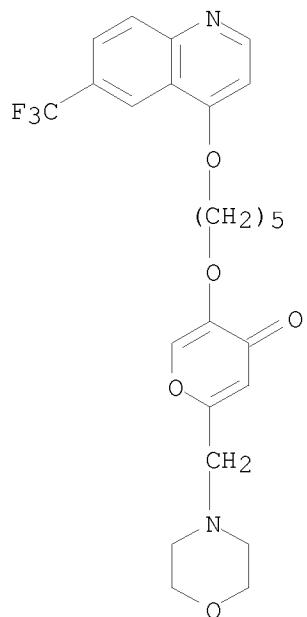
RN 754239-82-2 HCAPLUS

CN 4H-Pyran-4-one, 2-[(diethylamino)methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]- (CA INDEX NAME)



RN 754239-83-3 HCAPLUS

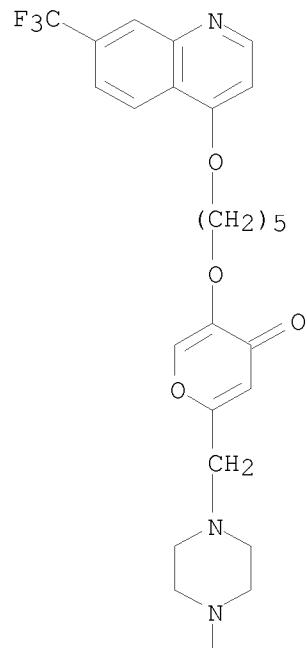
CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[6-(trifluoromethyl)-4-quinolinyl]oxy]pentyl]oxy]- (CA INDEX NAME)



RN 754239-84-4 HCAPLUS

CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]oxy]pentyl]oxy]- (CA INDEX NAME)

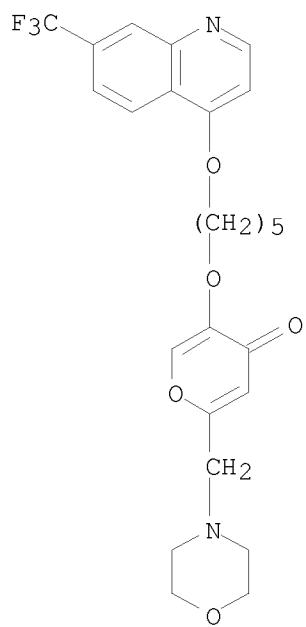
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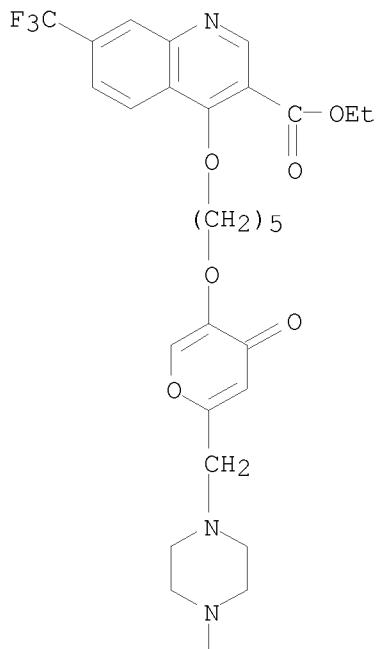
RN 754239-85-5 HCPLUS
CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]oxy]pentyl]oxy]- (CA INDEX NAME)



RN 754239-86-6 HCAPLUS

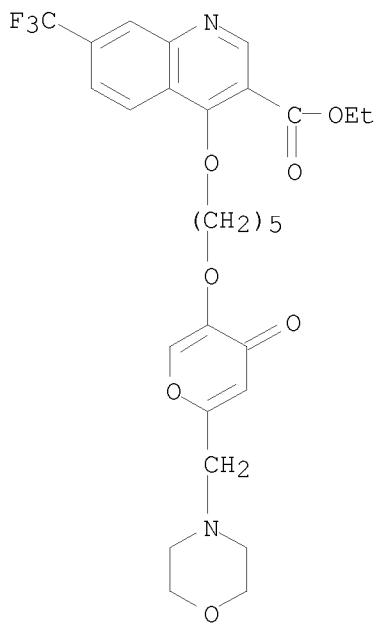
CN 3-Quinolincarboxylic acid, 4-[[5-[[6-[(4-methyl-1-piperazinyl)methyl]-4-oxo-4H-pyran-3-yl]oxy]pentyl]oxy]-7-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)

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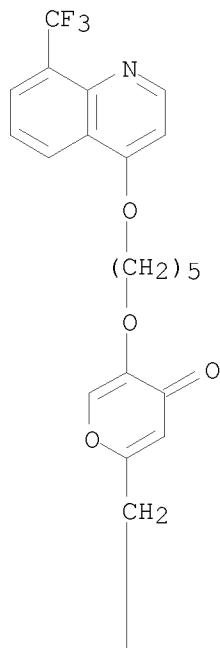
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Me

RN 754239-87-7 HCAPLUS
 CN 3-Quinolinecarboxylic acid, 4-[[5-[[6-(4-morpholinylmethyl)-4-oxo-4H-pyran-3-yl]oxy]pentyl]oxy]-7-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)

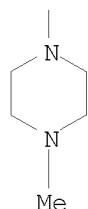


RN 754239-88-8 HCAPLUS
 CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[[5-[[8-(trifluoromethyl)-4-quinolinyl]oxy]pentyl]oxy]- (CA INDEX NAME)

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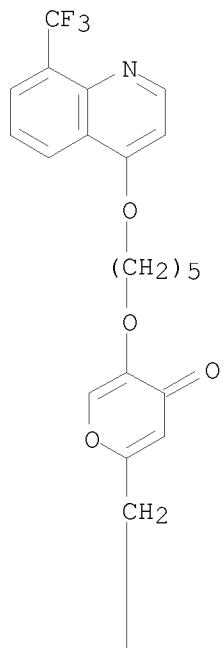
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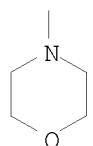
RN 754239-89-9 HCPLUS

CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[(5-[(8-(trifluoromethyl)-4-quinolinyl]oxy)pentyl]oxy]- (CA INDEX NAME)

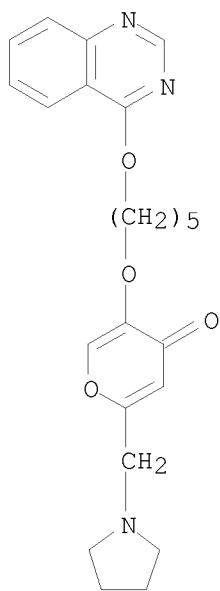
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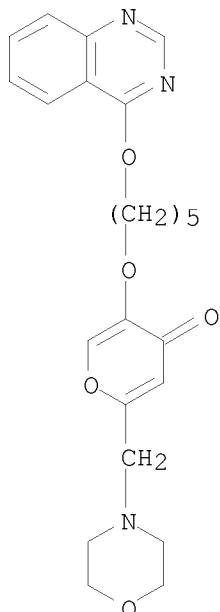


RN 754239-90-2 HCPLUS
CN 4H-Pyran-4-one, 2-(1-pyrrolidinylmethyl)-5-[5-(4-quinazolinyl)oxy]pentyl]oxy]- (CA INDEX NAME)



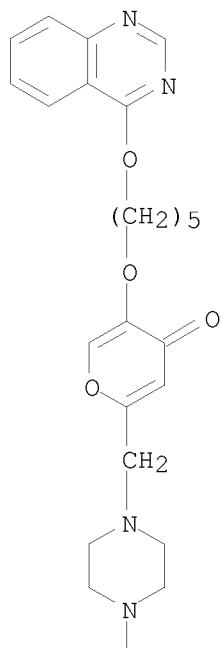
RN 754239-91-3 HCAPLUS

CN 4H-Pyran-4-one, 2-[(4-morpholinylmethyl)-5-[(5-(4-quinazolinylloxy)pentyl]oxy]pentyl]oxy- (CA INDEX NAME)

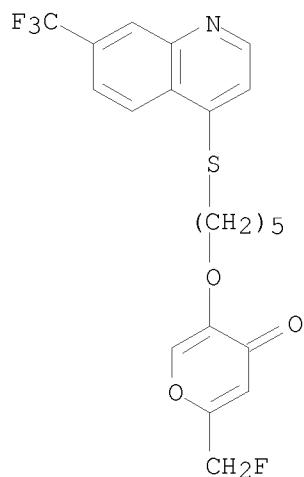


RN 754239-92-4 HCAPLUS

CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[(5-(4-quinazolinylloxy)pentyl]oxy]pentyl]oxy- (CA INDEX NAME)



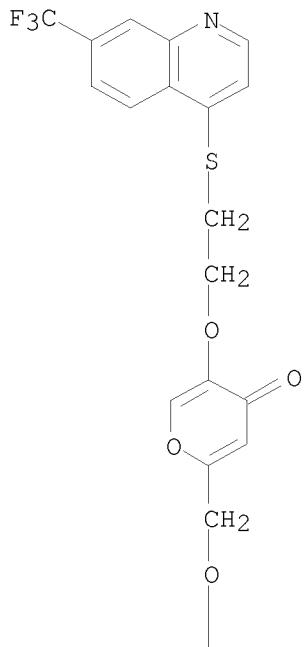
RN 754239-93-5 HCAPLUS
CN 4H-Pyran-4-one, 2-(fluoromethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



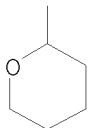
RN 754240-07-8 HCPLUS

CN 4H-Pyran-4-one, 2-[(2-[(2-(4-fluorobutyl)thio)ethyl]methyl]trifluoromethyl)-4-quinolinyl- (CA INDEX NAME)

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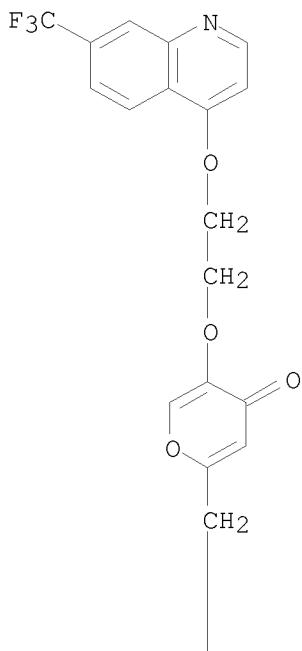
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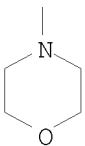
RN 754240-08-9 HCAPLUS

CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[2-[7-(trifluoromethyl)-4-quinolinyl]oxy]ethoxy- (CA INDEX NAME)

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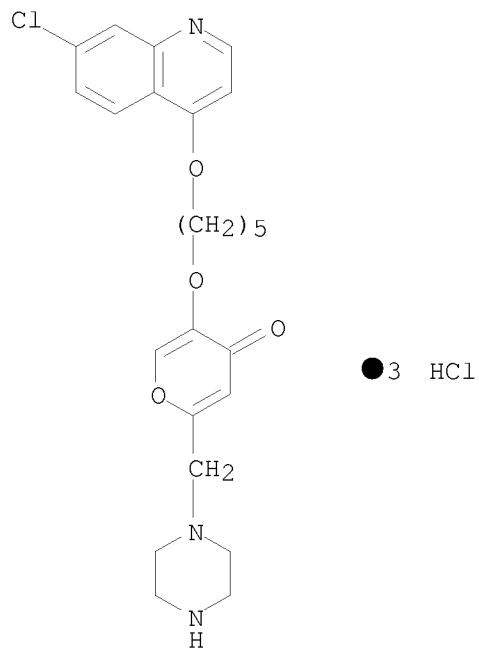


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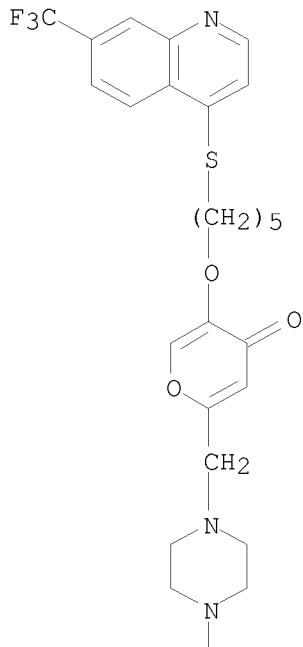
RN 754240-18-1 HCAPLUS

CN 4H-Pyran-4-one, 5-[5-[(7-chloro-4-quinolinyl)oxy]pentyl]oxy]-2-(1-piperazinylmethyl)-, hydrochloride (1:3) (CA INDEX NAME)



RN 754240-21-6 HCAPLUS
 CN 4H-Pyran-4-one, 2-[(4-acetyl-1-piperazinyl)methyl]-5-[[5-[[7-
 (trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)

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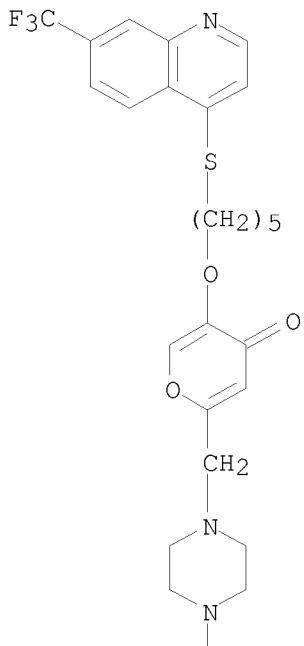
PAGE 2-A



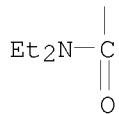
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CN 1-Piperazinecarboxamide, N,N-diethyl-4-[[4-oxo-5-[[5-[[7-(trifluoromethyl)-4-quinoliny]thio]pentyl]oxy]-4H-pyran-2-yl]methyl]- (CA INDEX NAME)

PAGE 1-A



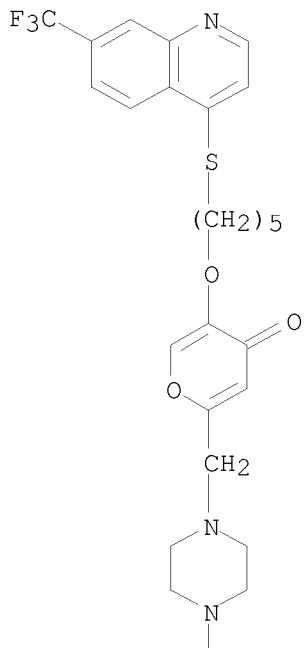
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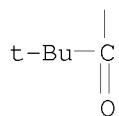
RN 754240-23-8 HCAPLUS

CN 4H-Pyran-4-one, 2-[[4-(2,2-dimethyl-1-oxopropyl)-1-piperazinyl]methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinoliny]thio]pentyl]oxy]- (CA INDEX NAME)

PAGE 1-A

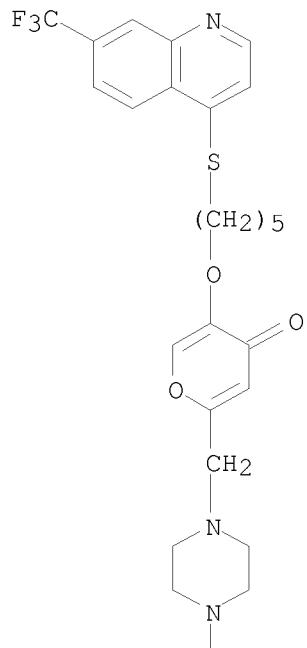


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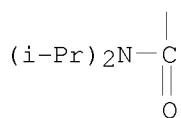


RN 754240-24-9 HCAPLUS
 CN 1-Piperazinecarboxamide, N,N-bis(1-methylethyl)-4-[4-oxo-5-[5-[7-(trifluoromethyl)-4-quinolinyl]thiopentyl]oxy]-4H-pyran-2-yl]methyl]-
 (CA INDEX NAME)

PAGE 1-A



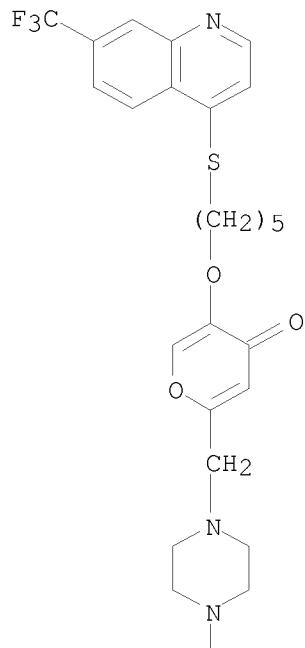
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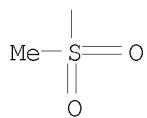
RN 754240-25-0 HCPLUS

CN 4H-Pyran-4-one, 2-[4-(methylsulfonyl)-1-piperazinylmethyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)

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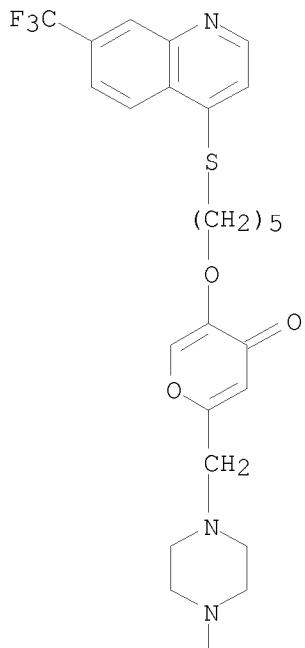


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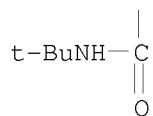


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 (CA INDEX NAME)

PAGE 1-A

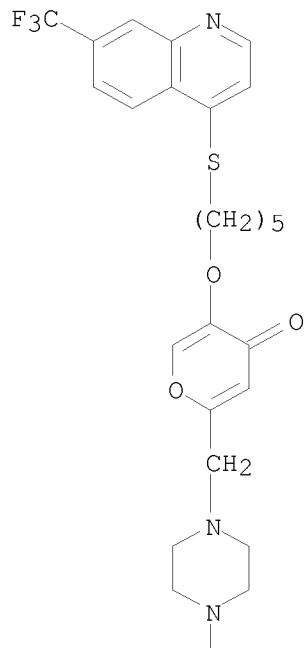


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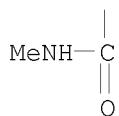


RN 754240-27-2 HCPLUS
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PAGE 1-A

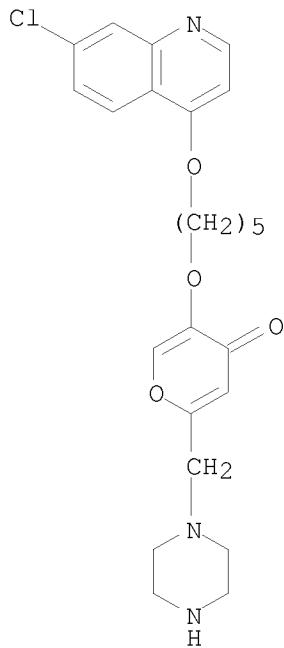


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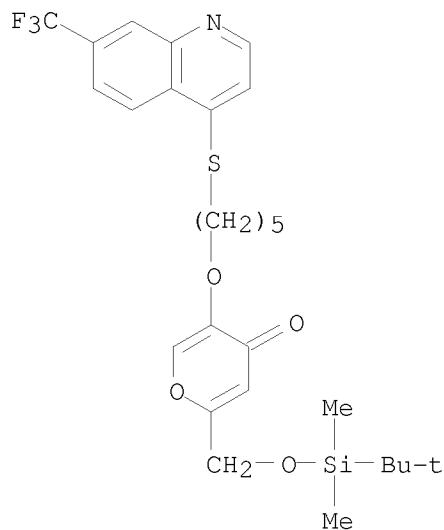


RN 754240-28-3 HCPLUS

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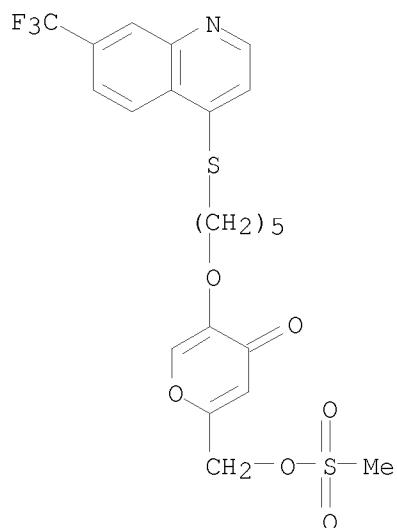


IT	754239-58-2P, 2-[(tert-Butyldimethylsilyloxy)methyl]-5-[[5-[[7-(trifluoromethyl)quinolin-4-yl]sulfanyl]pentyl]oxy]-4H-pyran-4-one 754239-61-7P, Methanesulfonic acid [4-oxo-5-[[5-(7-trifluoromethylquinolin-4-ylsulfanyl)pentyl]oxy]-4H-pyran-2-yl]methyl ester 754239-70-8P, 5-[[5-[6-(Trifluoromethyl)quinolin-4-yloxy]pentyl]oxy]-2-(hydroxymethyl)-4H-pyran-4-one 754239-71-9P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-yloxy]pentyl]oxy]-2-(hydroxymethyl)-4H-pyran-4-one 754239-72-0P, 4-[5-[(6-Hydroxymethyl-4-oxo-4H-pyran-3-yl)oxy]pentyloxy]-7-trifluoromethylquinoline-3-carboxylic acid ethyl ester 754239-73-1P, 5-[[5-[8-(Trifluoromethyl)quinolin-4-yloxy]pentyl]oxy]-2-(hydroxymethyl)-4H-pyran-4-one 754239-74-2P, 5-[[5-(Quinazolin-4-yloxy)pentyl]oxy]-2-(hydroxymethyl)-4H-pyran-4-one 754239-75-3P, [5-[[5-[6-(Trifluoromethyl)quinolin-4-yloxy]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl methanesulfonate 754239-76-4P, [5-[[5-[7-(Trifluoromethyl)quinolin-4-yloxy]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl methanesulfonate 754239-77-5P, 4-[[5-[(Methanesulfonyloxy)methyl]-4-oxo-4H-pyran-3-yl]oxy]pentyl]oxy]-7-trifluoromethylquinoline-3-carboxylic acid ethyl ester 754239-78-6P, [5-[[5-[8-(Trifluoromethyl)quinolin-4-yloxy]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl methanesulfonate 754239-79-7P, [5-[[5-(Quinazolin-4-yloxy)pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl methanesulfonate RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
RN	(intermediate; preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)
CN	754239-58-2 HCPLUS 4H-Pyran-4-one, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-5-[[5-[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



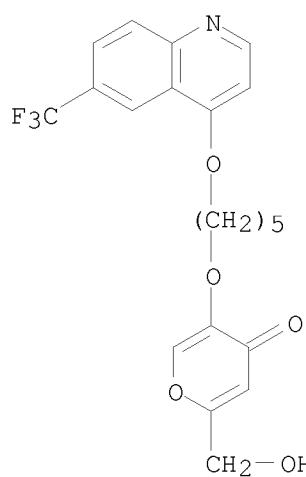
RN 754239-61-7 HCAPLUS

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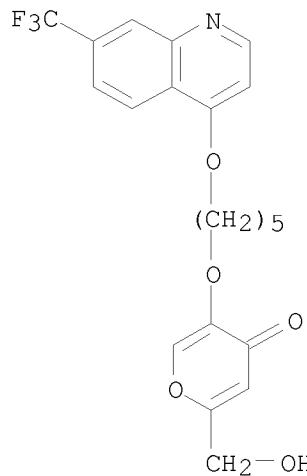
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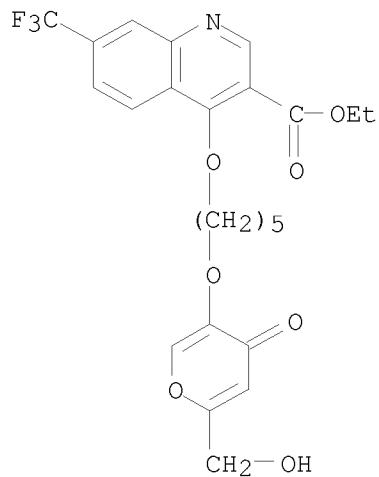
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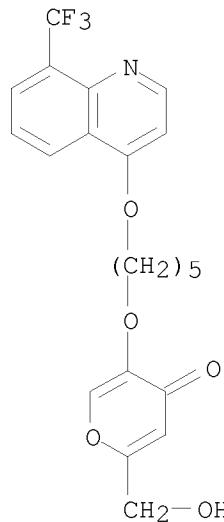
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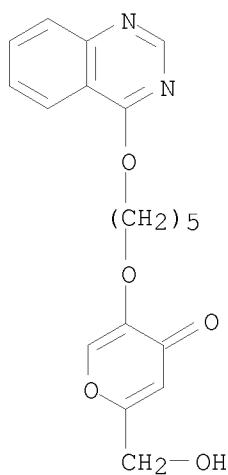
RN 754239-73-1 HCPLUS

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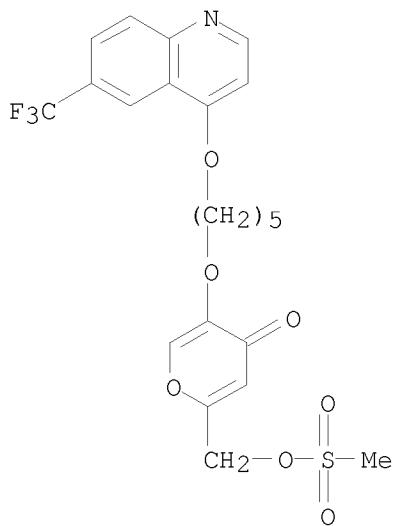
RN 754239-74-2 HCPLUS

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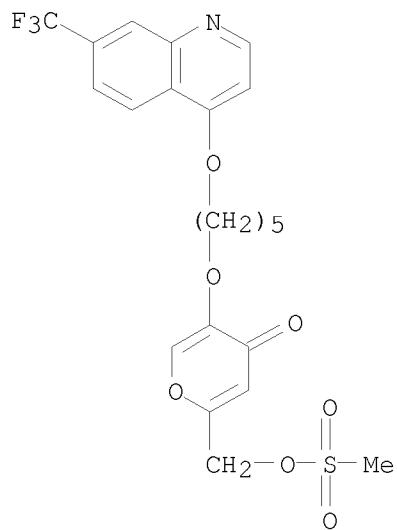
RN 754239-75-3 HCPLUS

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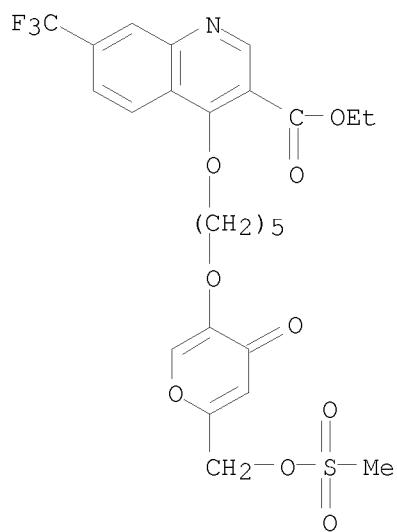
RN 754239-76-4 HCPLUS

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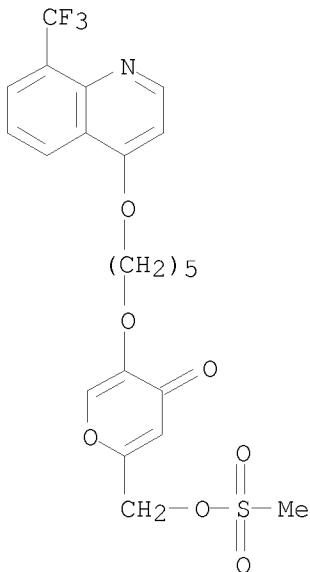
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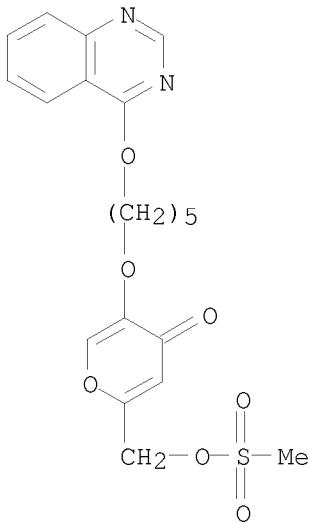
RN 754239-78-6 HCAPLUS

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RN 754239-79-7 HCAPLUS

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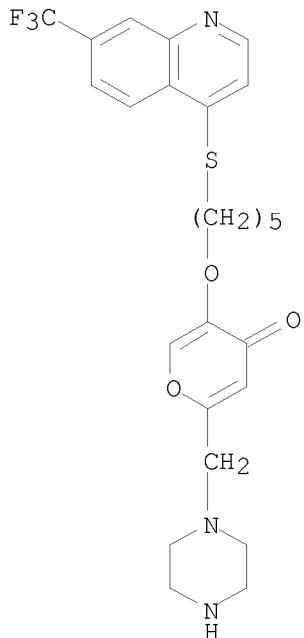
IT 754240-20-5, 5-[(5-[(7-(trifluoromethyl)quinolin-4-ylthio)pentyl]oxy)-2-[(piperazin-1-yl)methyl]-4H-pyran-4-one

RL: RCT (Reactant); RACT (Reactant or reagent)

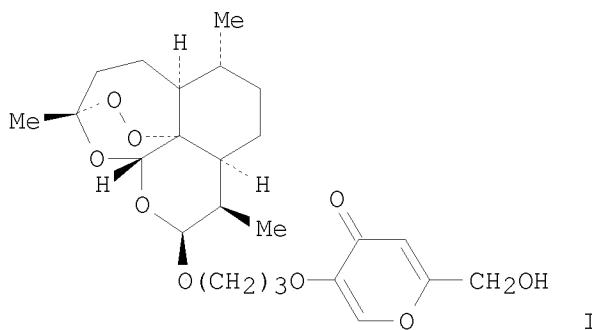
(preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)

RN 754240-20-5 HCAPLUS

CN 4H-Pyran-4-one, 2-(1-piperazinylmethyl)-5-[(5-[(7-(trifluoromethyl)-4-quinolinyl)thio]pentyl)oxy]- (CA INDEX NAME)



L4 ANSWER 5 OF 5 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:608133 HCPLUS
DOCUMENT NUMBER: 123:83751
ORIGINAL REFERENCE NO.: 123:15005a,15008a
TITLE: Mechanism-Based Development of New Antimalarials:
Synthesis of Derivatives of Artemisinin Attached to
Iron Chelators
AUTHOR(S): Kamchonwongpaisan, Sumalee; Paitayatat, Sumpan;
Thebtaranonth, Yodhathai; Wilairat, Prapin; Yuthavong,
Yongyuth
CORPORATE SOURCE: Faculty of Science, Mahidol University, Bangkok,
10400, Thailand
SOURCE: Journal of Medicinal Chemistry (1995), 38(13), 2311-16
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



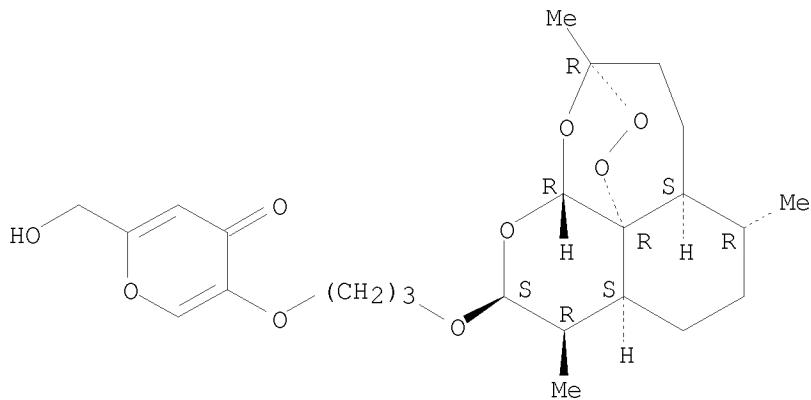
AB Various derivs. of artemisinin covalently linked to iron chelators, e.g. I, were synthesized, and their antimalarial activities were evaluated. Although results show no indication that the presence of an iron chelator in the vicinity of artemisinin potentiates its action, the linked compds. prepared still retain comparable activities to that of artemisinin.

IT 165068-36-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (mechanism-based development of new antimalarials, synthesis of derivs. of artemisinin attached to iron chelators)

RN 165068-36-0 HCPLUS

CN 4H-Pyran-4-one, 3-[3-[(decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyran-4-yl)oxy]propoxy]-6-(hydroxymethyl)-, [3R-(3 α ,5a β ,6 β ,8a β ,9 α ,10 α ,12 β ,12aR*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



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10541328

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DICTIONARY FILE UPDATES: 2 AUG 2008 HIGHEST RN 1037774-47-2

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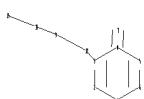
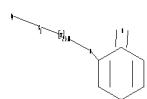
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ring nodes :
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chain bonds :
3-12 4-7 9-10 9-12 10-15

10541328

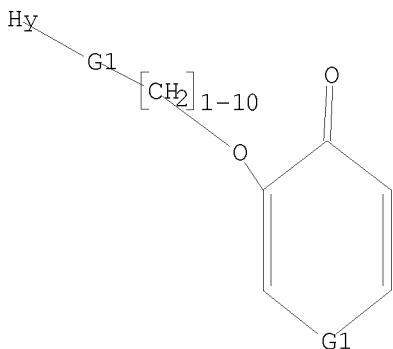
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exact/norm bonds :
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isolated ring systems :
containing 1 :

G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:Atom 12:CLASS
15:Atom

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L6 STR



G1 O,S,N

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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
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PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

10541328

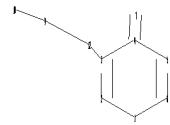
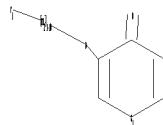
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100.0% PROCESSED 575864 ITERATIONS
SEARCH TIME: 00.00.08

85 ANSWERS

L8 85 SEA SSS FUL L6

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ring nodes :

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chain bonds :

3-12 4-7 9-10 9-12

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exact/norm bonds :

1-2 1-6 2-3 3-4 3-12 4-5 4-7 5-6 9-10 9-12

isolated ring systems :

containing 1 :

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Match level :

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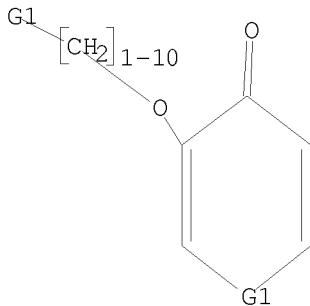
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L9 HAS NO ANSWERS

10541328

L9 STR



G1 O, S, N

Structure attributes must be viewed using STN Express query preparation.

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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 556571 TO 576709
PROJECTED ANSWERS: 58 TO 508

L10 1 SEA SSS SAM L9

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FULL SCREEN SEARCH COMPLETED - 575864 TO ITERATE

100.0% PROCESSED 575864 ITERATIONS 218 ANSWERS
SEARCH TIME: 00.00.04

L11 218 SEA SSS FUL L9

=> FIL HCAPLUS
COST IN U.S. DOLLARS SINCE FILE TOTAL
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CA SUBSCRIBER PRICE 0.00 -4.00

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FILE COVERS 1907 - 4 Aug 2008 VOL 149 ISS 6
FILE LAST UPDATED: 3 Aug 2008 (20080803/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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L5 1 S L4 AND PY<=2003

FILE 'REGISTRY' ENTERED AT 10:46:19 ON 04 AUG 2008

L6 STRUCTURE UPLOADED
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L8 85 S L6 SSS FULL
L9 STRUCTURE UPLOADED
L10 1 S L9
L11 218 S L9 SSS FULL

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=> s 115 and p/dt
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L16 11 L15 AND P/DT

=> s 116 and us/pc
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L17 5 L16 AND US/PC

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L12 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:622524 HCAPLUS

TITLE: Characterization of EHT 1864, a novel small molecule

inhibitor of Rac family small GTPases

AUTHOR(S): Onesto, Cercina; Shutes, Adam; Picard, Virginie;
Schweighoffer, Fabien; Der, Channing J.CORPORATE SOURCE: Lineberger Comprehensive Cancer Center, Department of
Pharmacology, University of North Carolina at Chapel
Hill, Chapel Hill, NC, USASOURCE: Methods in Enzymology (2008), 439 (Small GTPases in
Disease, Part B), 111-129

CODEN: MENZAU; ISSN: 0076-6879

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

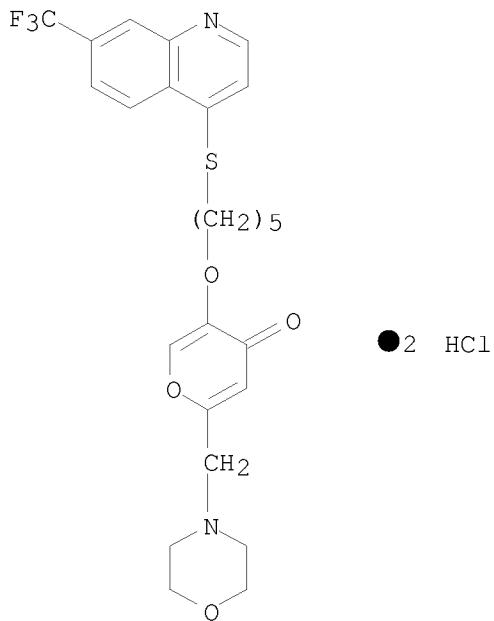
AB A review. There is now considerable exptl. evidence that aberrant activation of Rho family small GTPases promotes uncontrolled proliferation, invasion, and metastatic properties of human cancer cells. Therefore, there is considerable interest in the development of small mol. inhibitors of Rho GTPase function. However, to date, most efforts have focused on inhibitors that block Rho GTPase function indirectly, either by targeting enzymes involved in post-translational processing or downstream protein kinase effectors. We have reported the identification and characterization of the EHT 1864 small mol. as an inhibitor of Rac family small GTPases, placing Rac1 in an inert and inactive state and then impairing Rac1-mediated functions in vivo. Our work suggests that EHT 1864 selectively inhibits Rac1 downstream signaling and cellular transformation by a novel mechanism involving guanine nucleotide displacement. This chapter provides the details for some of the biochem. and biol. methods used to characterize the mode of action of EHT 1864 on Rac1 and its impact on Rac1-dependent cellular functions.

IT 754240-09-0, EHT1864

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU
(Therapeutic use); BIOL (Biological study); USES (Uses)
(biochem. and biol. methods may be useful to characterize Rho GTPase
specificity and mechanism of action of EHT 1864 on Rac1 and its impact
on Rac1-dependent cellular function in mouse)

RN 754240-09-0 HCAPLUS

CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-
quinolinyl]thio]pentyloxy]-, hydrochloride (1:2) (CA INDEX NAME)



L12 ANSWER 2 OF 6 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1368320 HCPLUS
DOCUMENT NUMBER: 148:232138
TITLE: Specificity and Mechanism of Action of EHT 1864, a Novel Small Molecule Inhibitor of Rac Family Small GTPases
AUTHOR(S): Shutes, Adam; Onesto, Cercina; Picard, Virginie; Leblond, Bertrand; Schweighoffer, Fabien; Der, Channing J.
CORPORATE SOURCE: Lineberger Comprehensive Cancer Center, University of North Carolina, Chapel Hill, NC, 27599, USA
SOURCE: Journal of Biological Chemistry (2007), 282(49), 35666-35678
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB There is now considerable exptl. evidence that aberrant activation of Rho family small GTPases promotes the uncontrolled proliferation, invasion, and metastatic properties of human cancer cells. Therefore, there is considerable interest in the development of small mol. inhibitors of Rho GTPase function. However, to date, most efforts have focused on inhibitors that indirectly block Rho GTPase function, by targeting either enzymes involved in post-translational processing or downstream protein kinase effectors. We recently determined that the EHT 1864 small mol. can inhibit Rac function *in vivo*. In this study, we evaluated the biol. and biochem. specificities and biochem. mechanism of action of EHT 1864. We determined that EHT 1864 specifically inhibited Rac1-dependent platelet-derived growth factor-induced lamellipodia formation. Furthermore, our biochem. analyses with recombinant Rac proteins found that EHT 1864 possesses high

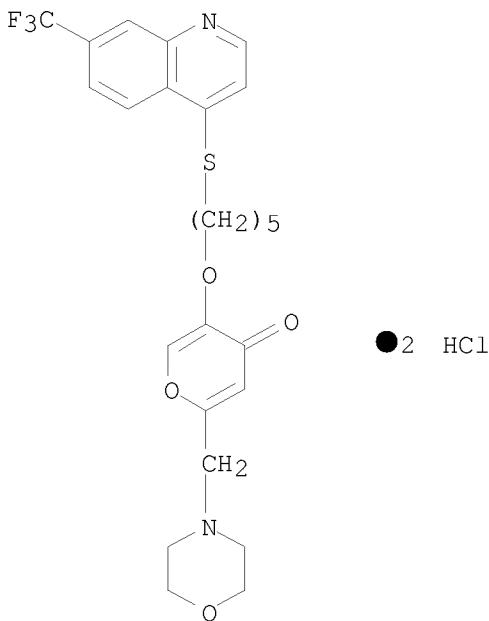
affinity binding to Rac1, as well as the related Rac1b, Rac2, and Rac3 isoforms, and this association promoted the loss of bound nucleotide, inhibiting both guanine nucleotide association and Tiam1 Rac guanine nucleotide exchange factor-stimulated exchange factor activity in vitro. EHT 1864 therefore places Rac in an inert and inactive state, preventing its engagement with downstream effectors. Finally, we evaluated the ability of EHT 1864 to block Rac-dependent growth transformation, and we determined that EHT 1864 potently blocked transformation caused by constitutively activated Rac1, as well as Rac-dependent transformation caused by Tiam1 or Ras. Taken together, our results suggest that EHT 1864 selectively inhibits Rac downstream signaling and transformation by a novel mechanism involving guanine nucleotide displacement.

IT 754240-09-0, EHT 1864

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(EHT 1864 specifically inhibits Rac1-dependent platelet-derived growth factor-induced lamellipodia formation)

RN 754240-09-0 HCPLUS

CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]-, hydrochloride (1:2) (CA INDEX NAME)



REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 6 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:525951 HCPLUS

DOCUMENT NUMBER: 147:143245

TITLE: Chemotherapy of leishmaniasis. Part V: Synthesis and in vitro bioevaluation of novel pyridinone derivatives

AUTHOR(S): Pandey, Susmita; Suryawanshi, S. N.; Nishi; Goyal, Neena; Gupta, Suman

CORPORATE SOURCE: Division of Medicinal Chemistry, Central Drug Research Institute, Lucknow, Uttar Pradesh, 226001, India

SOURCE: European Journal of Medicinal Chemistry (2007), 42(5), 669-674

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:143245

AB Alkylation of 3-hydroxy-2-methyl-4H-pyran-4-one with 1,5-dibromopentane gave dimeric γ -pyrone (2), which was recyclized with substituted anilines or cyclohexylamine to yield 1,1'-diaryl-2,2'-dimethyl-3,3'-pentamethylenedioxy-4,4'-bipyridinones (3a,b, d-j; aryl = 2,6-Me₂C₆H₃, 2,3-Me₂C₆H₃, 4-MeOC₆H₄, Ph, PhCH₂, 4-FC₆H₄, 4-ClC₆H₄, 4-NO₂C₆H₄, 2-MeOC₆H₄) and 1,1'-dicyclohexyl derivative (3c), together with the corresponding pyridinone-pyrone derivs., 1-Ar-2-methyl-3-[5-(2-methyl-4-oxo-4H-pyran-3-yloxy)pentyl]oxy]-4(4H)-pyridinones (4a-j, same Ar). The novel 2-substituted pyridinone derivs. were screened towards *in vitro* for their activity against leishmania antipromastigote and antimastigote activity profile, exhibiting good activity in some cases (3a, 3b; aryl = 2,6-Me₂C₆H₃, 2,3-Me₂C₆H₃, 4i, 4j, Ar = 4-NO₂C₆H₄, 2-MeOC₆H₄).

IT 943737-55-1P 943737-57-3P 943737-59-5P

943737-61-9P 943737-63-1P 943737-64-2P

943737-66-4P 943737-68-6P 943737-70-0P

943737-72-2P 943737-74-4P 943737-76-6P

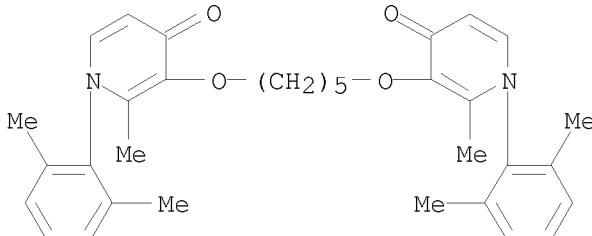
943737-77-7P 943737-79-9P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antileishmaniasis activity; preparation of pentamethylenedioxy-bridged bis-4-pyridinones and pyridinone-pyrone as antimicrobial agents against leishmaniasis)

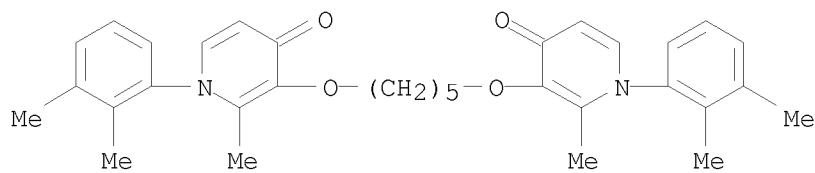
RN 943737-55-1 HCAPLUS

CN 4(1H)-Pyridinone, 3,3'-(1,5-pentanediylbis(oxy))bis[1-(2,6-dimethylphenyl)-2-methyl- (CA INDEX NAME)



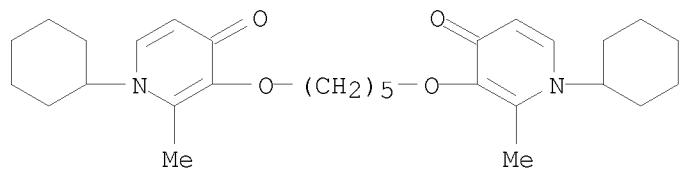
RN 943737-57-3 HCAPLUS

CN 4(1H)-Pyridinone, 3,3'-(1,5-pentanediylbis(oxy))bis[1-(2,3-dimethylphenyl)-2-methyl- (CA INDEX NAME)



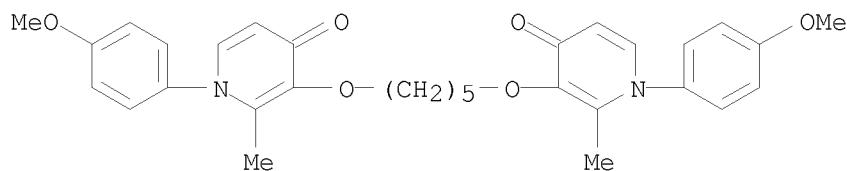
RN 943737-59-5 HCAPLUS

CN 4(1H)-Pyridinone, 3,3'-[1,5-pentanediylbis(oxy)]bis[1-cyclohexyl-2-methyl-4(1H)-pyridinone] (CA INDEX NAME)



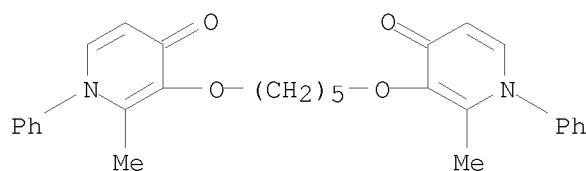
RN 943737-61-9 HCAPLUS

CN 4(1H)-Pyridinone, 3,3'-[1,5-pentanediylbis(oxy)]bis[1-(4-methoxyphenyl)-2-methyl-4(1H)-pyridinone] (CA INDEX NAME)



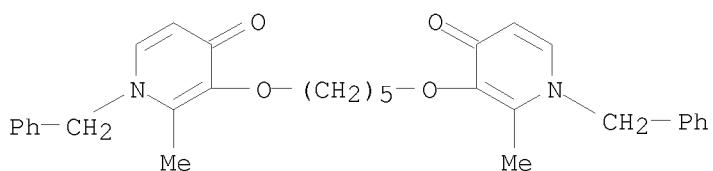
RN 943737-63-1 HCAPLUS

CN 4(1H)-Pyridinone, 3,3'-[1,5-pentanediylbis(oxy)]bis[2-methyl-1-phenyl-4(1H)-pyridinone] (CA INDEX NAME)

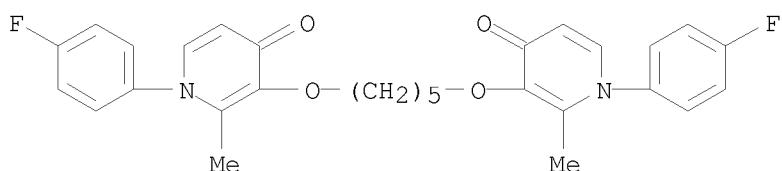


RN 943737-64-2 HCAPLUS

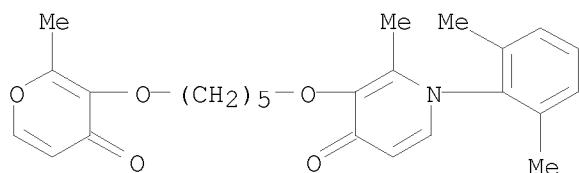
CN 4(1H)-Pyridinone, 3,3'-[1,5-pentanediylbis(oxy)]bis[2-methyl-1-(phenylmethyl)-4(1H)-pyridinone] (CA INDEX NAME)



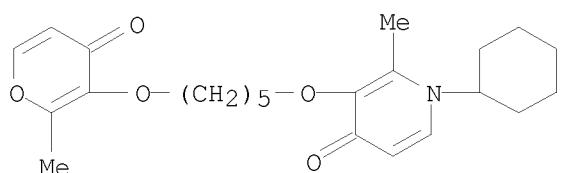
RN 943737-66-4 HCAPLUS
 CN 4(1H)-Pyridinone, 3,3'-[1,5-pentanediylibis(oxy)]bis[1-(4-fluorophenyl)-2-methyl- (CA INDEX NAME)]



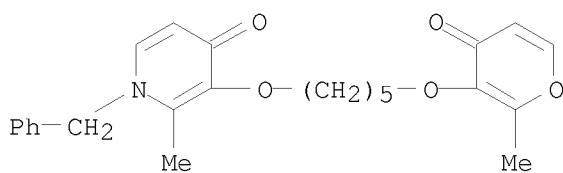
RN 943737-68-6 HCAPLUS
 CN 4(1H)-Pyridinone, 1-(2,6-dimethylphenyl)-2-methyl-3-[5-[(2-methyl-4-oxo-4H-pyran-3-yl)oxy]pentyl]oxy- (CA INDEX NAME)



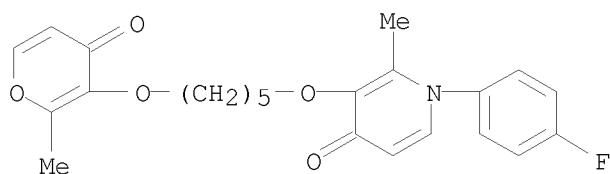
RN 943737-70-0 HCAPLUS
 CN 4(1H)-Pyridinone, 1-cyclohexyl-2-methyl-3-[5-[(2-methyl-4-oxo-4H-pyran-3-yl)oxy]pentyl]oxy- (CA INDEX NAME)



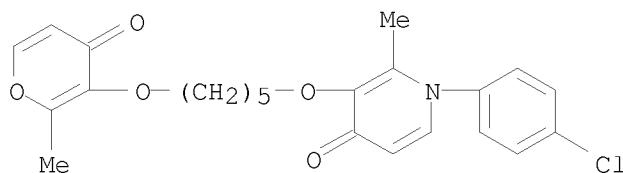
RN 943737-72-2 HCAPLUS
 CN 4(1H)-Pyridinone, 2-methyl-3-[5-[(2-methyl-4-oxo-4H-pyran-3-yl)oxy]pentyl]oxy-1-(phenylmethyl)- (CA INDEX NAME)



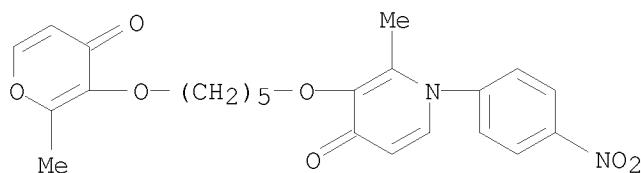
RN 943737-74-4 HCAPLUS
 CN 4(1H)-Pyridinone, 1-(4-fluorophenyl)-2-methyl-3-[5-[(2-methyl-4-oxo-4H-pyran-3-yl)oxy]pentyl]oxy- (CA INDEX NAME)



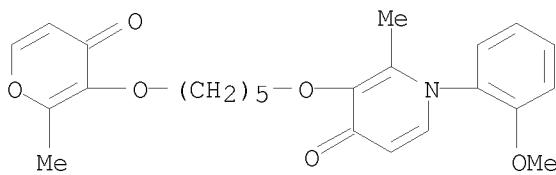
RN 943737-76-6 HCAPLUS
 CN 4(1H)-Pyridinone, 1-(4-chlorophenyl)-2-methyl-3-[5-[(2-methyl-4-oxo-4H-pyran-3-yl)oxy]pentyl]oxy- (CA INDEX NAME)



RN 943737-77-7 HCAPLUS
 CN 4(1H)-Pyridinone, 2-methyl-3-[5-[(2-methyl-4-oxo-4H-pyran-3-yl)oxy]pentyl]oxy]-1-(4-nitrophenyl)- (CA INDEX NAME)



RN 943737-79-9 HCAPLUS
 CN 4(1H)-Pyridinone, 1-(2-methoxyphenyl)-2-methyl-3-[5-[(2-methyl-4-oxo-4H-pyran-3-yl)oxy]pentyl]oxy- (CA INDEX NAME)



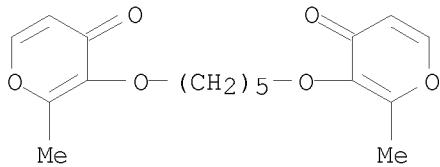
IT 943737-53-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pentamethylenedioxy-bridged bis-4-pyridinones and pyridinone-pyrone as antimicrobial agents against leishmaniasis)

RN 943737-53-9 HCPLUS

CN 4H-Pyran-4-one, 3,3'-[1,5-pentanediylbis(oxy)]bis[2-methyl- (CA INDEX NAME)



REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 6 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1191062 HCPLUS

DOCUMENT NUMBER: 144:68139

TITLE: RAC1 Inhibition Targets Amyloid Precursor Protein Processing by γ -Secretase and Decreases A β Production in Vitro and in Vivo

AUTHOR(S): Desire, Laurent; Bourdin, Jerome; Loiseau, Nadia; Peillon, Helene; Picard, Virginie; De Oliveira, Catherine; Bachelot, Florence; Leblond, Bertrand; Taverne, Thierry; Beausoleil, Eric; Lacombe, Sandrine; Drouin, Dominique; Schweighoffer, Fabien

CORPORATE SOURCE: Exonhit Therapeutics, Paris, 75013, Fr.
SOURCE: Journal of Biological Chemistry (2005), 280(45), 37516-37525CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular BiologyDOCUMENT TYPE: Journal
LANGUAGE: EnglishAB β -Amyloid peptides (A β) that form the senile plaques of Alzheimer disease consist mainly of 40- and 42-amino acid (A β 40 and A β 42) peptides generated from the cleavage of the amyloid precursor protein (APP). Generation of A β involves β -secretase and γ -secretase activities and is regulated by membrane trafficking of the proteins involved in A β production. Here we describe a new small mol., EHT 1864, which blocks the Rac1 signaling pathways. In vitro, EHT 1864 blocks A β 40 and A β 42 production but does not impact

sAPP α levels and does not inhibit β -secretase. Rather, EHT 1864 modulates APP processing at the level of γ -secretase to prevent A β 40 and A β 42 generation. This effect does not result from a direct inhibition of the γ -secretase activity and is specific for APP cleavage, since EHT 1864 does not affect Notch cleavage. In vivo, EHT 1864 significantly reduces A β 40 and A β 42 levels in guinea pig brains at a threshold that is compatible with delaying plaque accumulation and/or clearing the existing plaque in brain. EHT 1864 is the first derivative of a new chemical series that consists of candidates for inhibiting A β formation in the brain of AD patients. Our findings represent the first pharmacol. validation of Rac1 signaling as a target for developing novel therapies for Alzheimer disease.

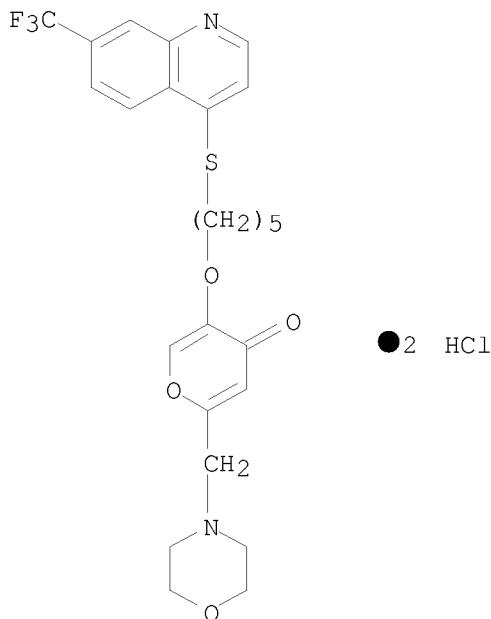
IT 754240-09-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(EHT 1864; EHT 1864 blocked A β 1-40 and A β 1-42 production)

RN 754240-09-0 HCPLUS

CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]-, hydrochloride (1:2) (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 6 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:740320 HCPLUS

DOCUMENT NUMBER: 141:260557

TITLE: Preparation of novel antiproliferative and antiangiogenic agents, in particular

quinoline-derivatized pyranones, for treating cell

proliferative diseases, retinopathies and arthritis

INVENTOR(S): Leblond, Bertrand; Petit, Silvere; Picard, Virginie; Taverne, Thierry; Schweighoffer, Fabien

PATENT ASSIGNEE(S): Exonhit Therapeutics Sa, Fr.
 SOURCE: PCT Int. Appl., 156 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: English

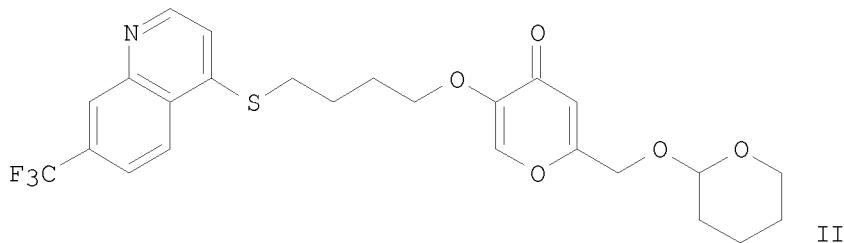
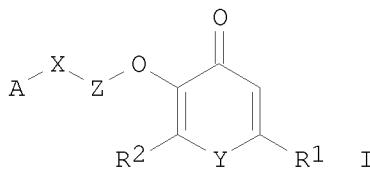
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004076445	A2	20040910	WO 2004-IB926	20040227
WO 2004076445	A3	20050106		
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AU 2004215577	A1	20040910	AU 2004-215577	20040227
CA 2516239	A1	20040910	CA 2004-2516239	20040227
EP 1597253	A2	20051123	EP 2004-715422	20040227
EP 1597253	B1	20060809		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1747952	A	20060315	CN 2004-80003820	20040227
JP 2006519221	T	20060824	JP 2006-502497	20040227
AT 335734	T	20060915	AT 2004-715422	20040227
US 20060183749	A1	20060817	US 2005-541328	20050830
PRIORITY APPLN. INFO.:			EP 2003-290490	A 20030228
			WO 2004-IB926	W 20040227

OTHER SOURCE(S): MARPAT 141:260557

GI



AB Title compds. I [wherein R1 = [(tetrahydropyran-2-yl)oxy]methyl, CH2-B, (morpholin-4-yl)methyl, pyrrolidin-1-ylmethyl, etc.; B = halo, OH, OCH2OMe, OCH2OCH2CH2OMe, OSO2-alkyl, OTBDMS; R2 = H, alk(en)yl; X, Y = independently O, S, NH and derivs.; A = quinolin-4-yl, quinolin-8-yl, benzo[b]thiophen-7-yl, quinazolin-4-yl; Z = (CH2)*n*, optionally interrupted by a heteroatom, C(:O) or aryldialkyl, especially xlenyl, group; *n* = 1-10; their tautomers, optical and geometrical isomers, racemates, salts, hydrates and mixts.] were prepared as antiproliferative agents and angiogenesis inhibitors. Nine biol. assays are given. For example, II was prepared, in 2 steps, from pyranone III, 1,4-dibromobutane, and 7-(trifluoromethyl)-4-quinolinethiol. In an in vitro cell viability assay, selected I showed an IC50 < 4 μ M and < 9 μ M against HCT116 and MDA-MB-231 tumoral cell lines, demonstrating their cytostatic mode of action. I are useful for treating various diseases associated with abnormal cell proliferation, including cancer, especially leukemia, or associated with unregulated angiogenesis including growth and metastasis of solid tumors, ocular diseases, especially retinopathies, or arthritis.

IT 754240-09-0P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-(morpholinomethyl)-4H-pyran-4-one dihydrochloride
 754240-17-0P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-[(4-methylpiperazin-1-yl)methyl]-4H-pyran-4-one trihydrochloride 754240-19-2P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-[(piperazin-1-yl)methyl]-4H-pyran-4-one trihydrochloride

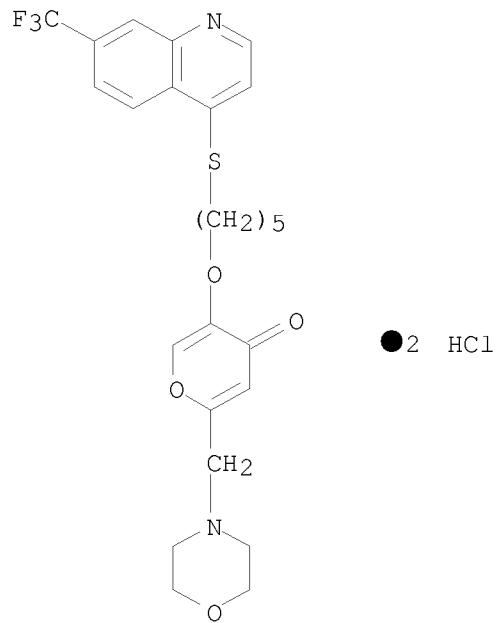
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)

RN 754240-09-0 HCAPLUS

CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[7-(trifluoromethyl)-4-

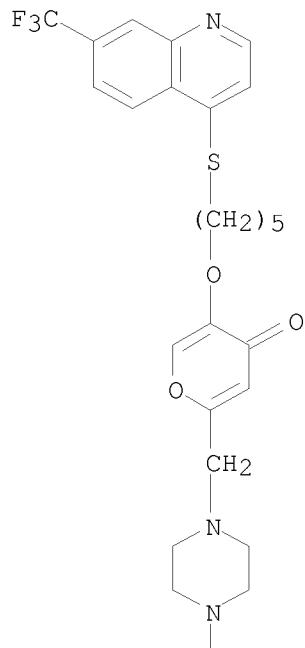
10541328

quinolinyl]thio]pentyl]oxy]-, hydrochloride (1:2) (CA INDEX NAME)



RN 754240-17-0 HCPLUS
CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[[5-[(7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-, hydrochloride (1:3) (CA INDEX NAME)

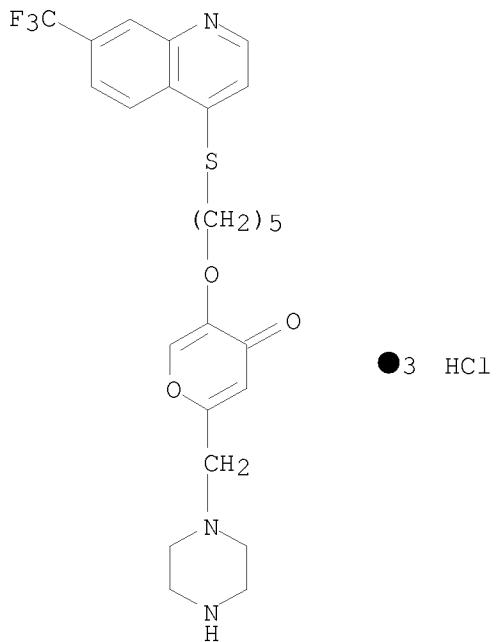
PAGE 1-A



PAGE 2-A

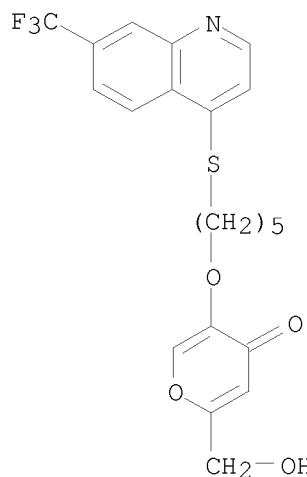
●3 HCl

RN 754240-19-2 HCPLUS
CN 4H-Pyran-4-one, 2-(1-piperazinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thiopentyl]oxy]-, hydrochloride (1:3) (CA INDEX NAME)



IT 754239-59-3P, 2-Hydroxymethyl-5-[[5-[7-(trifluoromethyl)quinolin-4-ylsulfanyl]pentyl]oxy]-4H-pyran-4-one 754240-15-8P, tert-Butyl 4-[[5-[[5-[7-(trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]piperazine-1-carboxylate 754240-16-9P, tert-Butyl 4-[[5-[[5-(7-chloroquinolin-4-yloxy)pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]piperazine-1-carboxylate
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate; preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)

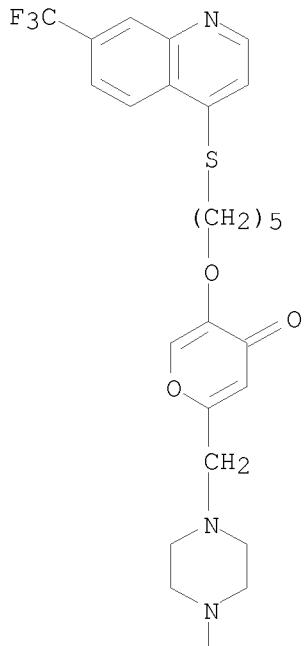
RN 754239-59-3 HCAPLUS
 CN 4H-Pyran-4-one, 2-(hydroxymethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



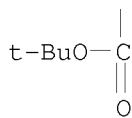
RN 754240-15-8 HCPLUS

CN 1-Piperazinecarboxylic acid, 4-[[4-oxo-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-4H-pyran-2-yl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

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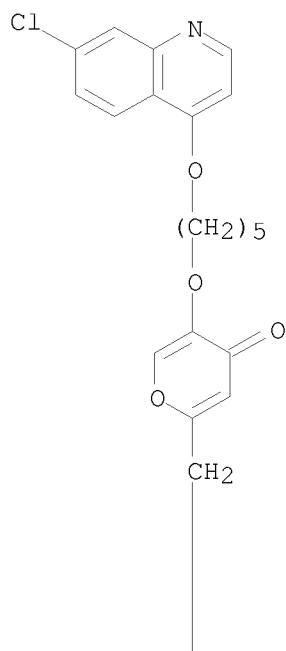
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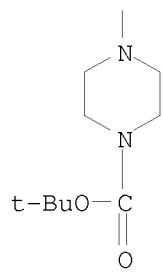
RN 754240-16-9 HCPLUS

CN 1-Piperazinecarboxylic acid, 4-[[5-[[5-[(7-chloro-4-quinolinyloxy]pentyloxy]-4-oxo-4H-pyran-2-yl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

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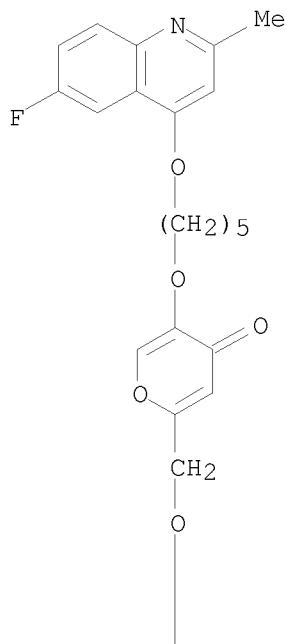
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, 5-[[5-(6-Fluoro-2-trifluoromethylquinolin-4-yloxy)pentyl]oxy]-2-
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 5-[[5-(7-Propylquinolin-8-yloxy)pentyl]oxy]-2-[[[(tetrahydropyran-2-
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 2-[[[(Tetrahydropyran-2-yl)oxy]methyl]-5-[4-[[7-(trifluoromethyl)quinolin-4-
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 4H-pyran-4-one hydrochloride 754239-60-6P, 2-
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 4-[[5-[[6-(4-Methylpiperazin-1-ylmethyl)-4-oxo-4H-pyran-3-
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 ester 754239-87-7P, 4-[[5-[[6-[(Morpholin-4-yl)methyl]-4-oxo-4H-
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 ethyl ester 754239-88-8P, 5-[[5-[8-(Trifluoromethyl)quinolin-4-
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 754239-89-9P, 5-[[5-[8-(Trifluoromethyl)quinolin-4-
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 , 5-[[5-(Quinazolin-4-yloxy)pentyl]oxy]-2-[(pyrrolidin-1-yl)methyl]-4H-
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(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-[(4-acetylpirazin-1-yl)methyl]-4H-pyran-4-one 754240-22-7P, 4-[[5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]-N,N-diethylpirazin-1-carboxamide 754240-23-8P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-[(4-(pivaloyl)piperazin-1-yl)methyl]-4H-pyran-4-one 754240-24-9P, 4-[[5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]-N,N-diisopropylpirazin-1-carboxamide 754240-25-0P, 5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-2-[(4-Methylsulfonylpiperazin-1-yl)methyl]-4H-pyran-4-one 754240-26-1P, 4-[[5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]-N-tert-butylpiperazin-1-carboxamide 754240-27-2P, 4-[[5-[[5-[7-(Trifluoromethyl)quinolin-4-ylthio]pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl]-N-methylpirazin-1-carboxamide 754240-28-3P, 5-[[5-(7-Chloroquinolin-4-yl)oxy]pentyl]oxy]-2-[(piperazin-1-yl)methyl]-4H-pyran-4-one
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)

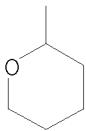
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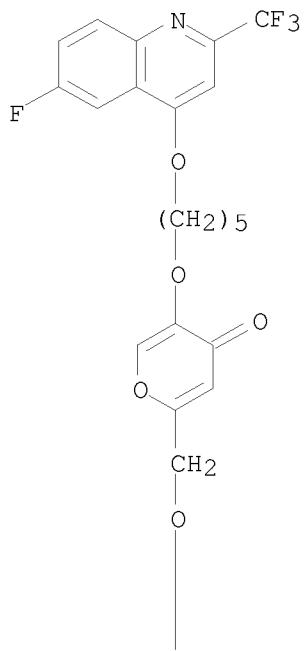
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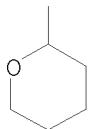
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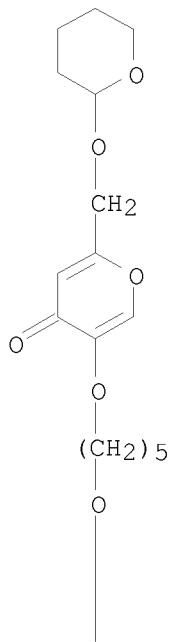


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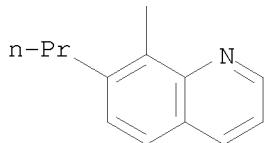
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10541328

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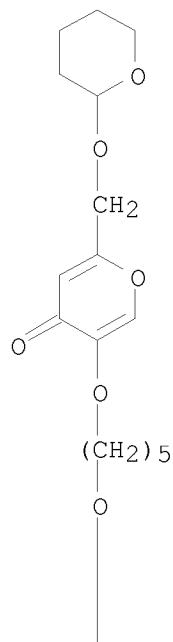


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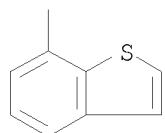


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CN 4H-Pyran-4-one, 5-[5-(benzo[b]thien-7-yloxy)pentyl]oxy]-2-[(tetrahydro-2H-pyran-2-yl)oxy]methyl- (CA INDEX NAME)

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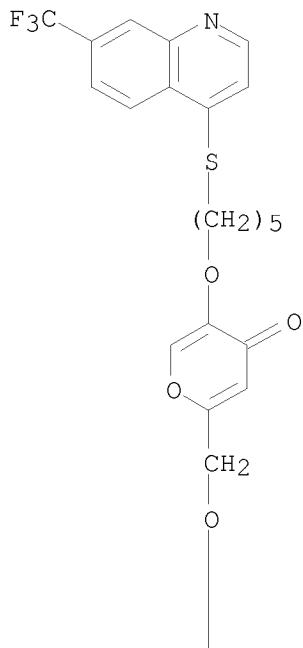


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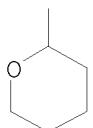


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CN 4H-Pyran-4-one, 2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thiopentyl]oxy]- (CA INDEX NAME)

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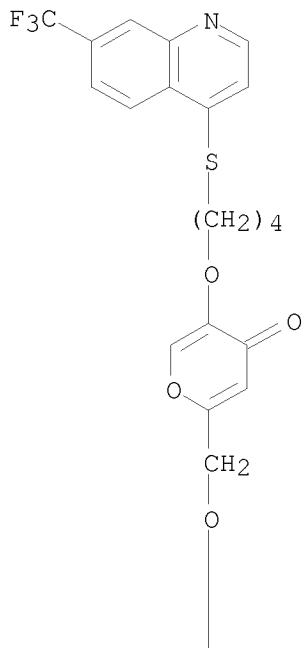
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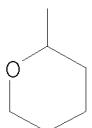
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CN 4H-Pyran-4-one, 2-[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[4-[(7-(trifluoromethyl)-4-quinolinylthio)butoxy]- (CA INDEX NAME)

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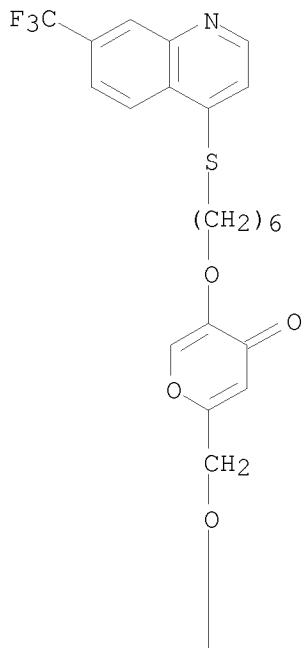


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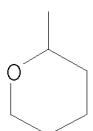


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CN 4H-Pyran-4-one, 2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[[6-[[7-(trifluoromethyl)-4-quinolinyl]thio]hexyl]oxy]- (CA INDEX NAME)

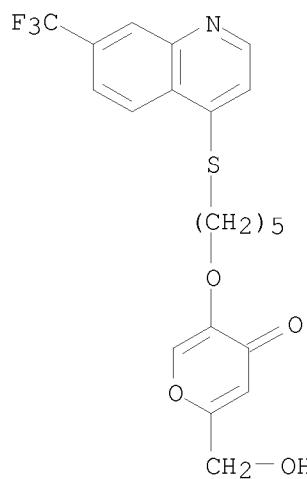
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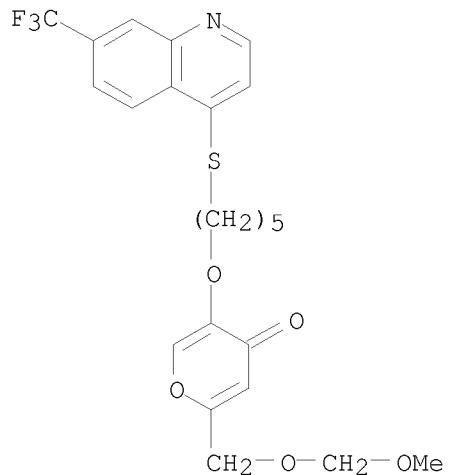
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CN 4H-Pyran-4-one, 2-(hydroxymethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

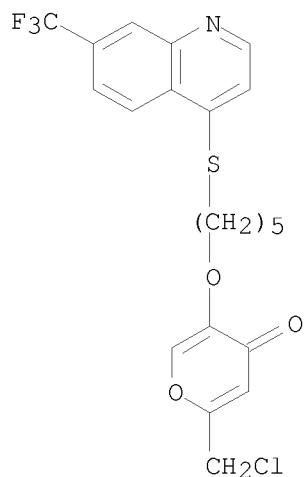
RN 754239-60-6 HCPLUS

CN 4H-Pyran-4-one, 2-[(methoxymethoxy)methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



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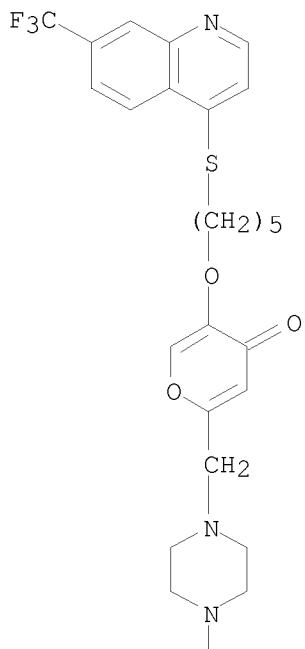
CN 4H-Pyran-4-one, 2-(chloromethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



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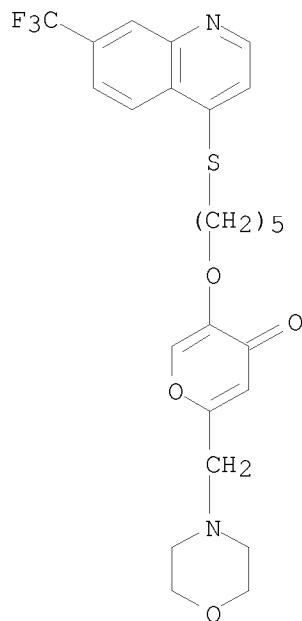
CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[[5-[(7-(trifluoromethyl)-4-quinolinyloxy)pentyl]thio]pentyl]oxy]- (CA INDEX NAME)

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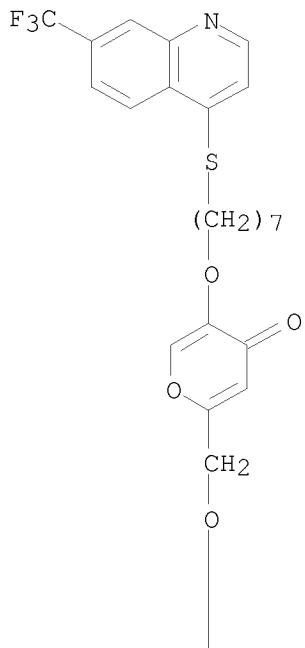
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RN 754239-64-0 HCAPLUS
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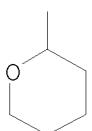


RN 754239-66-2 HCAPLUS
CN 4H-Pyran-4-one, 2-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-[[7-[[7-(trifluoromethyl)-4-quinolinyl]thio]heptyloxy]- (CA INDEX NAME)

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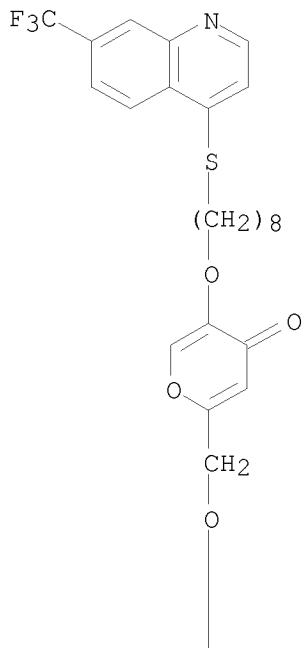


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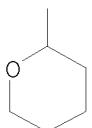


RN 754239-68-4 HCPLUS
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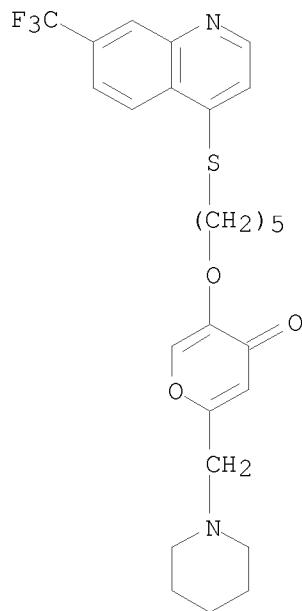
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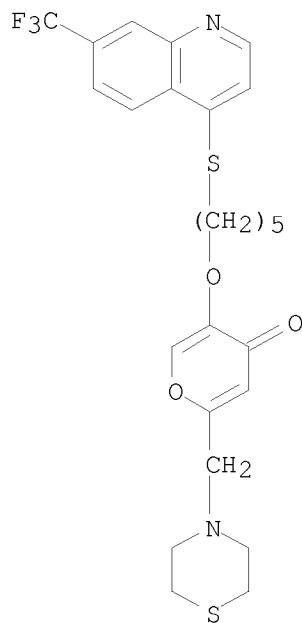


RN 754239-80-0 HCPLUS
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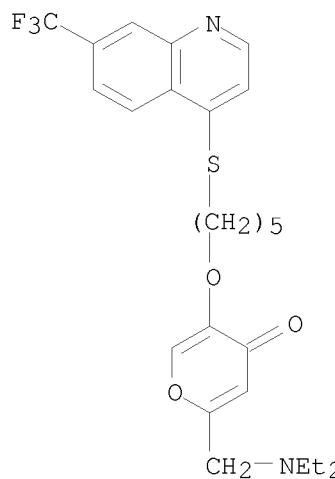
RN 754239-81-1 HCAPLUS

CN 4H-Pyran-4-one, 2-(4-thiomorpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]- (CA INDEX NAME)



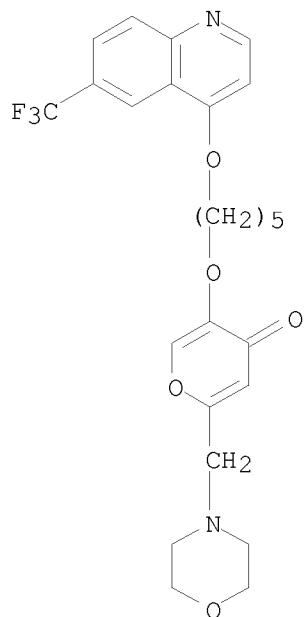
RN 754239-82-2 HCAPLUS

CN 4H-Pyran-4-one, 2-[(diethylamino)methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyloxy]- (CA INDEX NAME)



RN 754239-83-3 HCAPLUS

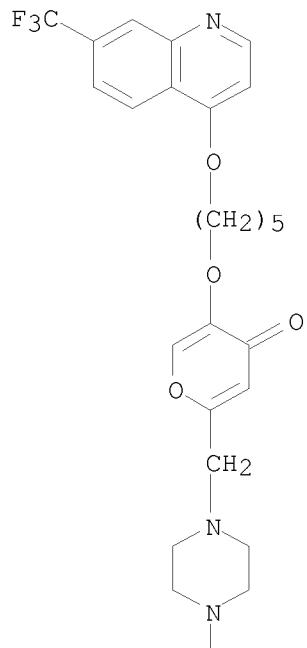
CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[6-(trifluoromethyl)-4-quinolinyl]oxy]pentyl]oxy]- (CA INDEX NAME)



RN 754239-84-4 HCAPLUS

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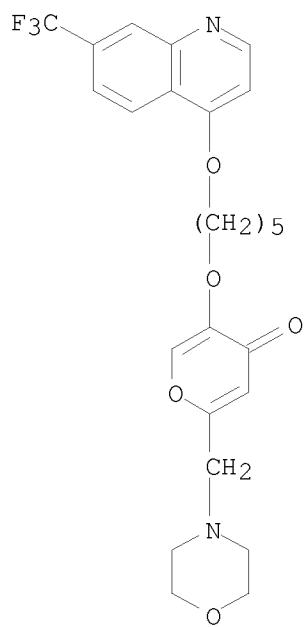
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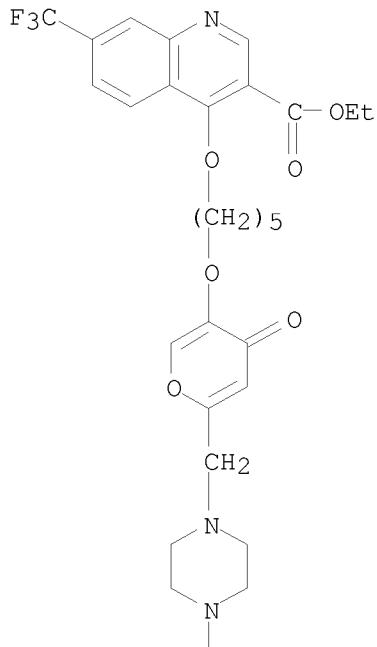
RN 754239-85-5 HCPLUS
CN 4H-Pyran-4-one, 2-(4-morpholinylmethyl)-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]oxy]pentyloxy]- (CA INDEX NAME)



RN 754239-86-6 HCAPLUS

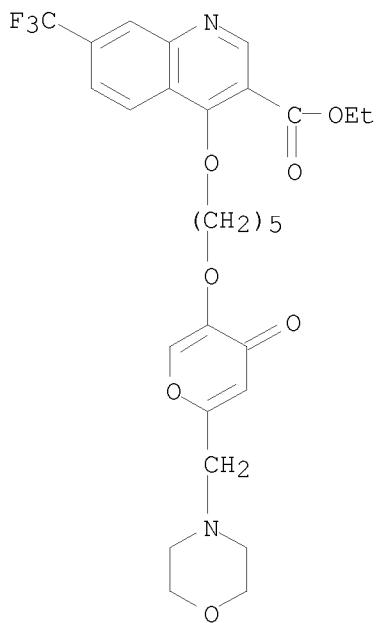
CN 3-Quinolincarboxylic acid, 4-[[5-[[6-[(4-methyl-1-piperazinyl)methyl]-4-oxo-4H-pyran-3-yl]oxy]pentyl]oxy]-7-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)

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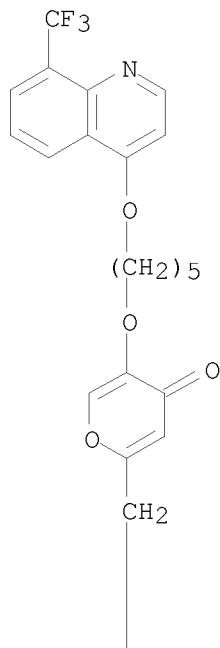
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RN 754239-87-7 HCAPLUS
 CN 3-Quinolinecarboxylic acid, 4-[[5-[[6-(4-morpholinylmethyl)-4-oxo-4H-pyran-3-yl]oxy]pentyl]oxy]-7-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)

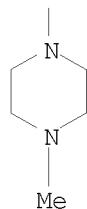


RN 754239-88-8 HCAPLUS
 CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[[5-[[8-(trifluoromethyl)-4-quinoliny]oxy]pentyl]oxy]- (CA INDEX NAME)

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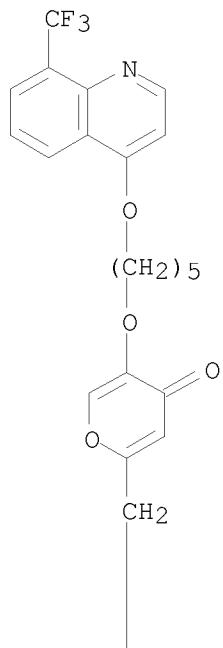
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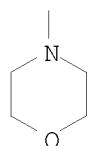
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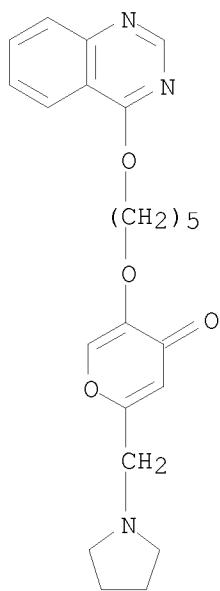
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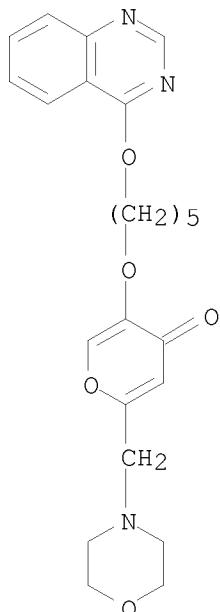


RN 754239-90-2 HCPLUS
CN 4H-Pyran-4-one, 2-(1-pyrrolidinylmethyl)-5-[5-(4-quinazolinyl)oxy]pentyl]oxy]- (CA INDEX NAME)



RN 754239-91-3 HCAPLUS

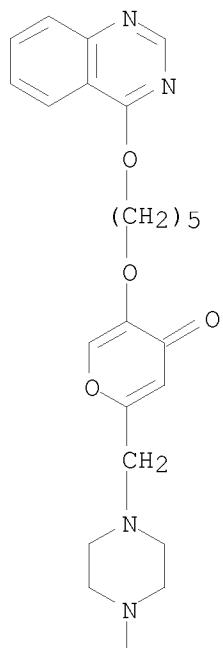
CN 4H-Pyran-4-one, 2-[(4-morpholinylmethyl)-5-[(5-(4-quinazolinyl)oxy)pentyl]oxy]- (CA INDEX NAME)



RN 754239-92-4 HCAPLUS

CN 4H-Pyran-4-one, 2-[(4-methyl-1-piperazinyl)methyl]-5-[(5-(4-quinazolinyl)oxy)pentyl]oxy]- (CA INDEX NAME)

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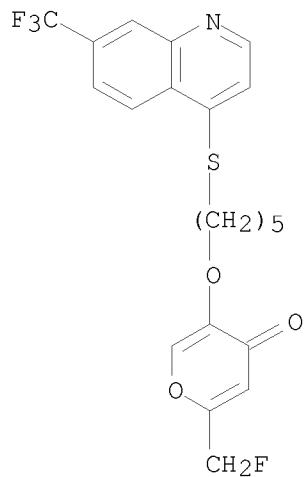


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RN 754239-93-5 HCAPLUS
CN 4H-Pyran-4-one, 2-(fluoromethyl)-5-[5-[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl- (CA INDEX NAME)

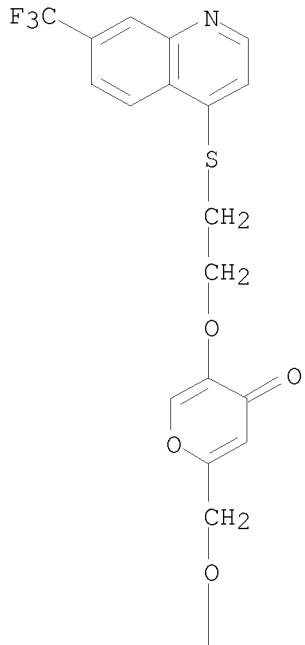
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RN 754240-07-8 HCPLUS

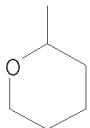
CN 4H-Pyran-4-one, 2-[(2-[(2-(4-fluorobutyl)thio)ethyl]methyl]trifluoromethyl)-4-quinolinyl]- (CA INDEX NAME)

PAGE 1-A



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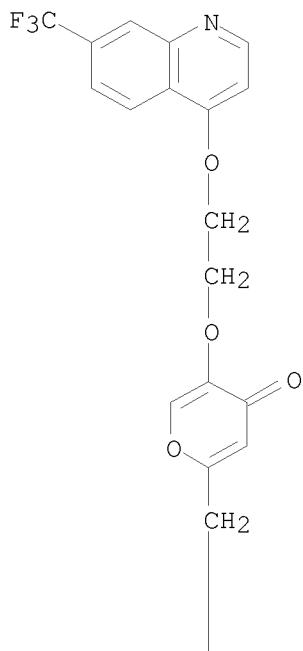
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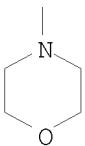
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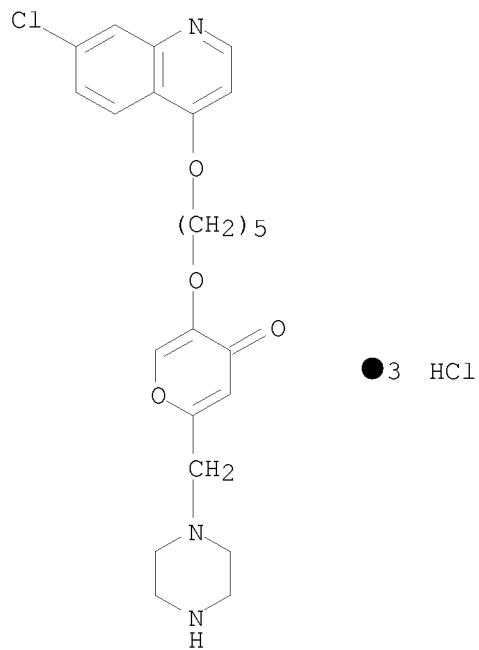


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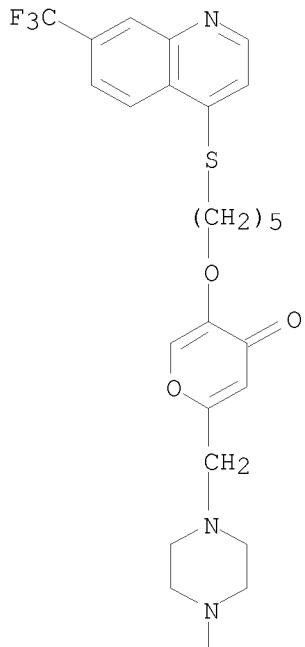
RN 754240-18-1 HCAPLUS

CN 4H-Pyran-4-one, 5-[5-[(7-chloro-4-quinolinyl)oxy]pentyl]oxy]-2-(1-piperazinylmethyl)-, hydrochloride (1:3) (CA INDEX NAME)



RN 754240-21-6 HCAPLUS
 CN 4H-Pyran-4-one, 2-[(4-acetyl-1-piperazinyl)methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)

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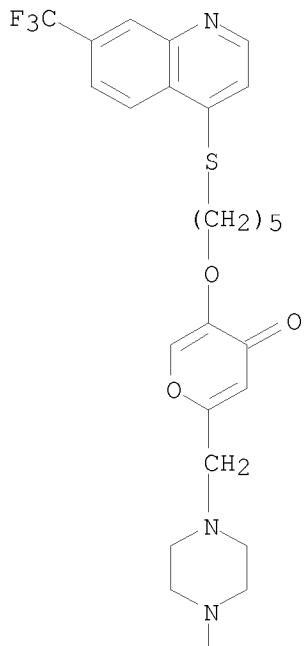
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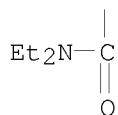
RN 754240-22-7 HCAPLUS

CN 1-Piperazinecarboxamide, N,N-diethyl-4-[[4-oxo-5-[[5-[[7-(trifluoromethyl)-4-quinoliny]thio]pentyl]oxy]-4H-pyran-2-yl]methyl]- (CA INDEX NAME)

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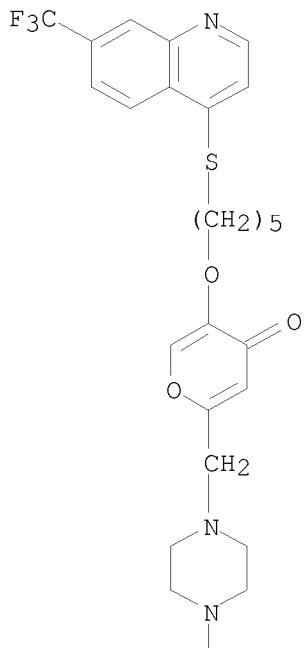
PAGE 2-A



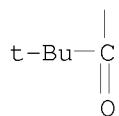
RN 754240-23-8 HCAPLUS

CN 4H-Pyran-4-one, 2-[[4-(2,2-dimethyl-1-oxopropyl)-1-piperazinyl]methyl]-5-[[5-[[7-(trifluoromethyl)-4-quinoliny]thio]pentyl]oxy]- (CA INDEX NAME)

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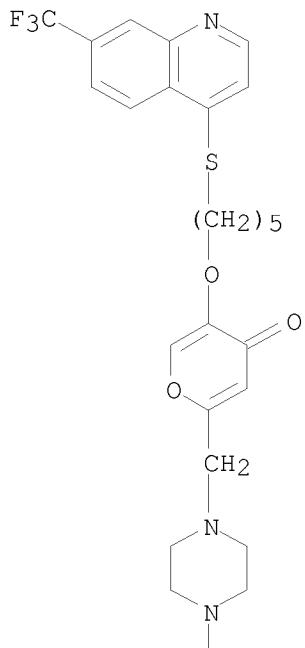


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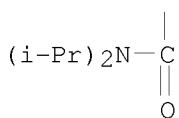


RN 754240-24-9 HCPLUS
 CN 1-Piperazinecarboxamide, N,N-bis(1-methylethyl)-4-[[4-oxo-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-4H-pyran-2-yl]methyl]-
 (CA INDEX NAME)

PAGE 1-A

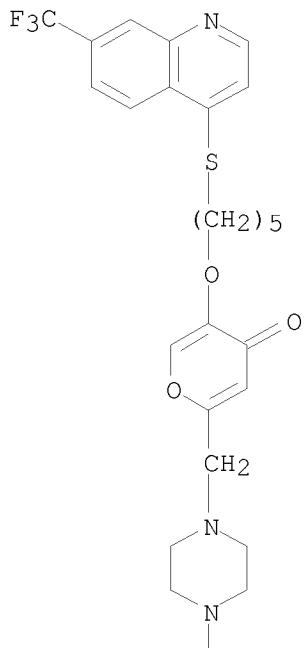


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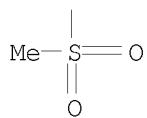


RN 754240-25-0 HCAPLUS
 CN 4H-Pyran-4-one, 2-[4-(methylsulfonyl)-1-piperazinylmethyl]-5-[[5-[[7-(trifluoromethyl)-4-quinoliny]thio]pentyl]oxy]- (CA INDEX NAME)

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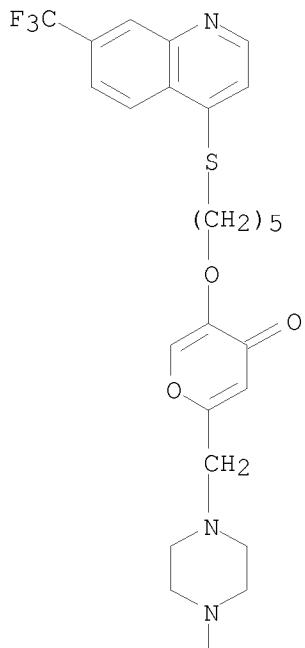


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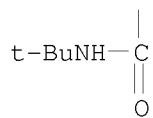


RN 754240-26-1 HCPLUS
 CN 1-Piperazinecarboxamide, N-(1,1-dimethylethyl)-4-[[4-oxo-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-4H-pyran-2-yl]methyl]-
 (CA INDEX NAME)

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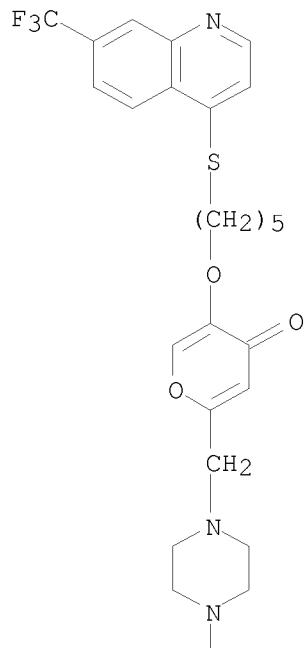


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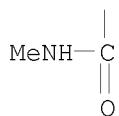


RN 754240-27-2 HCPLUS
 CN 1-Piperazinecarboxamide, N-methyl-4-[[4-oxo-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]-4H-pyran-2-yl]methyl]- (CA INDEX NAME)

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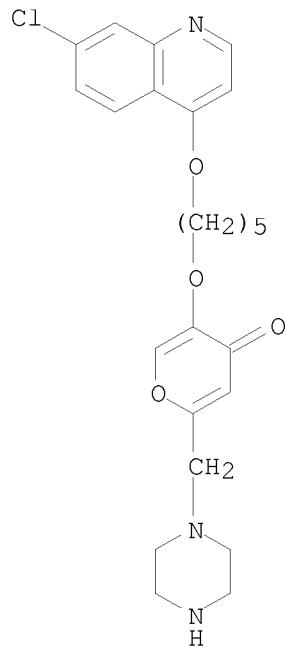


PAGE 2-A



RN 754240-28-3 HCPLUS

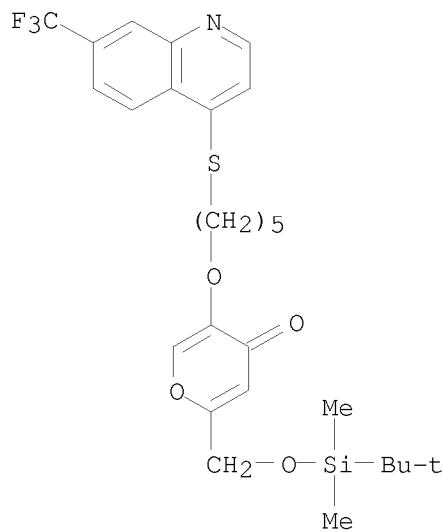
CN 4H-Pyran-4-one, 5-[[5-[(7-chloro-4-quinolinyloxy]pentyl]oxy]-2-(1-piperazinylmethyl)- (CA INDEX NAME)



IT 754239-58-2P, 2-[(tert-Butyldimethylsilyloxy)methyl]-5-[[5-[[7-(trifluoromethyl)quinolin-4-yl]sulfanyl]pentyl]oxy]-4H-pyran-4-one
 754239-61-7P, Methanesulfonic acid [4-oxo-5-[[5-[(7-trifluoromethyl)quinolin-4-yl]sulfanyl]pentyl]oxy]-4H-pyran-2-yl]methyl ester 754239-70-8P, 5-[[5-[(6-(Trifluoromethyl)quinolin-4-yloxy)pentyl]oxy]-2-(hydroxymethyl)-4H-pyran-4-one 754239-71-9P, 5-[[5-[(7-(Trifluoromethyl)quinolin-4-yloxy)pentyl]oxy]-2-(hydroxymethyl)-4H-pyran-4-one 754239-72-0P, 4-[[5-[(6-Hydroxymethyl-4-oxo-4H-pyran-3-yl)oxy]pentyl]oxy]-7-trifluoromethylquinoline-3-carboxylic acid ethyl ester 754239-73-1P, 5-[[5-[(8-(Trifluoromethyl)quinolin-4-yloxy)pentyl]oxy]-2-(hydroxymethyl)-4H-pyran-4-one 754239-74-2P, 5-[[5-[(Quinazolin-4-yloxy)pentyl]oxy]-2-(hydroxymethyl)-4H-pyran-4-one 754239-75-3P, 5-[[5-[(6-(Trifluoromethyl)quinolin-4-yloxy)pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl methanesulfonate 754239-76-4P, [5-[[5-[(7-(Trifluoromethyl)quinolin-4-yloxy)pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl methanesulfonate 754239-77-5P, 4-[[5-[(6-[(Methanesulfonyloxy)methyl]pentyl]oxy]-7-trifluoromethylquinoline-3-carboxylic acid ethyl ester 754239-78-6P, [5-[[5-[(8-(Trifluoromethyl)quinolin-4-yloxy)pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl methanesulfonate 754239-79-7P, [5-[[5-[(Quinazolin-4-yloxy)pentyl]oxy]-4-oxo-4H-pyran-2-yl]methyl methanesulfonate
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)

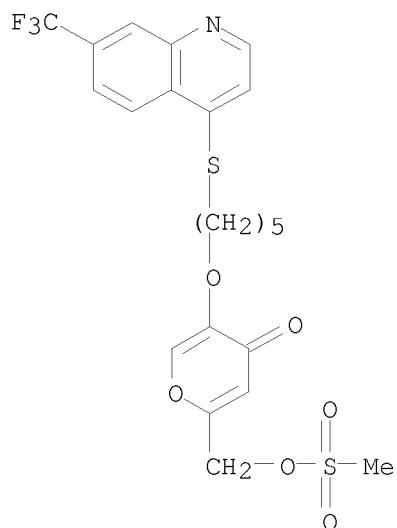
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CN 4H-Pyran-4-one, 2-[[[[1,1-dimethyl-ethyl]dimethylsilyl]oxy]methyl]-5-[[5-[(7-(trifluoromethyl)-4-quinolinyl)thio]pentyl]oxy]- (CA INDEX NAME)



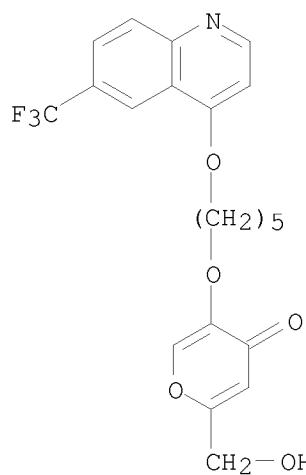
RN 754239-61-7 HCAPLUS

CN 4H-Pyran-4-one, 2-[(methylsulfonyl)oxy]methyl-5-[[5-[[7-(trifluoromethyl)-4-quinolinyl]thio]pentyl]oxy]- (CA INDEX NAME)



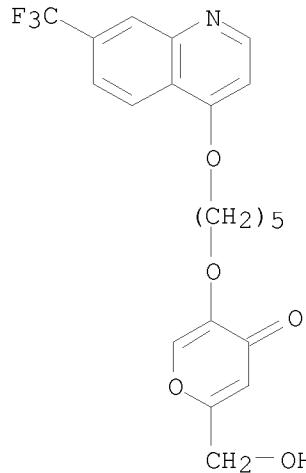
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CN 4H-Pyran-4-one, 2-(hydroxymethyl)-5-[[5-[[6-(trifluoromethyl)-4-quinolinyl]oxy]pentyl]oxy]- (CA INDEX NAME)



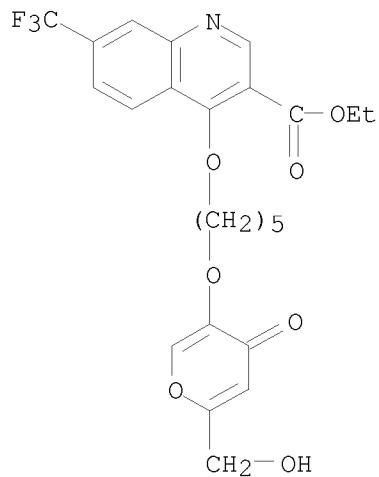
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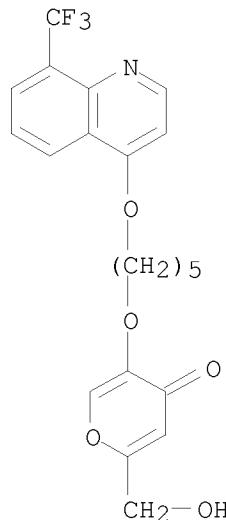
RN 754239-72-0 HCAPLUS

CN 3-Quinolinecarboxylic acid, 4-[[5-[[6-(hydroxymethyl)-4-oxo-4H-pyran-3-yl]oxy]pentyl]oxy]-7-(trifluoromethyl)-, ethyl ester (CA INDEX NAME)



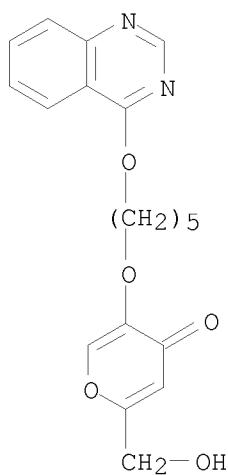
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CN 4H-Pyran-4-one, 2-(hydroxymethyl)-5-[5-[5-[8-(trifluoromethyl)-4-quinolinyl]oxy]pentyl]oxy]- (CA INDEX NAME)



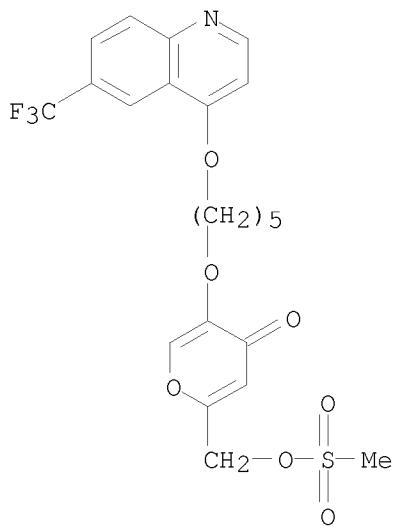
RN 754239-74-2 HCPLUS

CN 4H-Pyran-4-one, 2-(hydroxymethyl)-5-[5-[5-[4-quinazolinyl]oxy]pentyl]oxy]- (CA INDEX NAME)



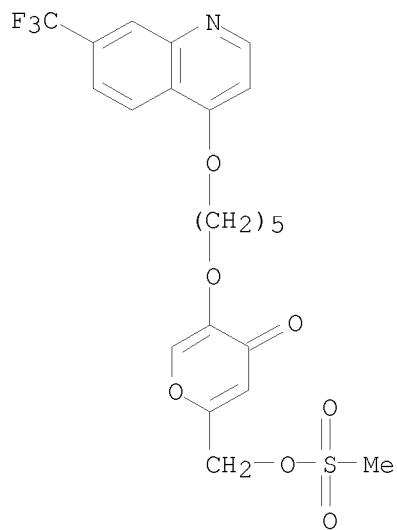
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CN 4H-Pyran-4-one, 2-[(methylsulfonyl)oxy]methyl]-5-[[5-[(6-(trifluoromethyl)-4-quinolinyloxy)pentyl]oxy]- (CA INDEX NAME)

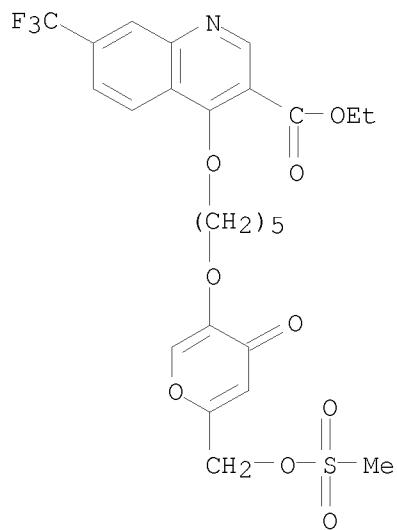


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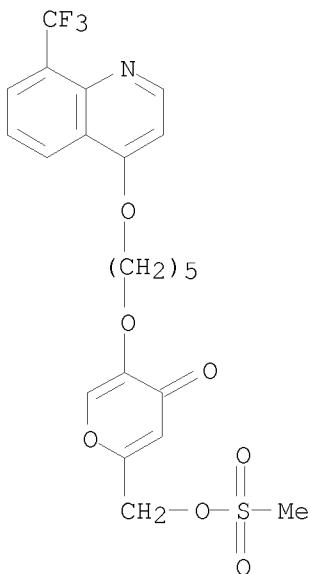
CN 4H-Pyran-4-one, 2-[(methylsulfonyl)oxy]methyl]-5-[[5-[(7-(trifluoromethyl)-4-quinolinyloxy)pentyl]oxy]- (CA INDEX NAME)



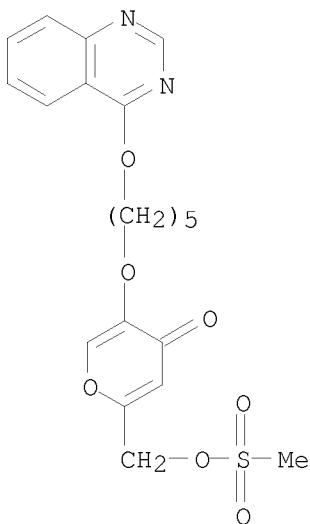
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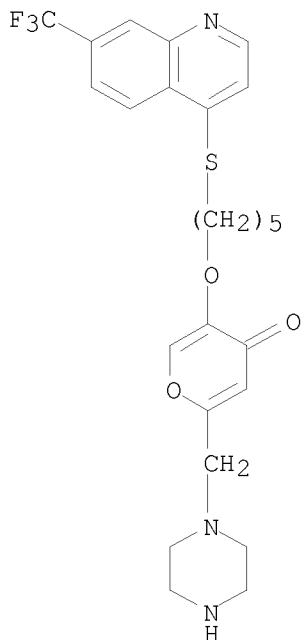
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RN 754239-79-7 HCAPLUS
 CN 4H-Pyran-4-one, 2-[(5-[(methylsulfonyl)oxy]methyl)-5-[(4-quinazolinyl)oxy]pentyl]oxy]- (CA INDEX NAME)



IT 754240-20-5, 5-[(5-[(7-(trifluoromethyl)quinolin-4-ylthio)pentyl]oxy)-2-[(piperazin-1-yl)methyl]-4H-pyran-4-one
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of novel antiproliferative and antiangiogenic agents, in particular quinoline-derivatized pyranones, for treating cell proliferative diseases, retinopathies and arthritis)
 RN 754240-20-5 HCAPLUS
 CN 4H-Pyran-4-one, 2-(1-piperazinylmethyl)-5-[(5-[(7-(trifluoromethyl)quinolinyl)thio]pentyl)oxy]- (CA INDEX NAME)



L12 ANSWER 6 OF 6 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:608133 HCPLUS

DOCUMENT NUMBER: 123:83751

ORIGINAL REFERENCE NO.: 123:15005a,15008a

TITLE: Mechanism-Based Development of New Antimalarials:
Synthesis of Derivatives of Artemisinin Attached to
Iron Chelators

AUTHOR(S): Kamchonwongpaisan, Sumalee; Paitayatat, Sumparn;
Thebtaranonth, Yodhathai; Wilairat, Prapin; Yuthavong,
Yongyuth

CORPORATE SOURCE: Faculty of Science, Mahidol University, Bangkok,
10400, Thailand

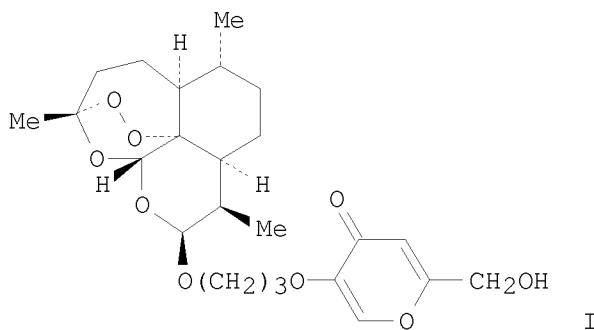
SOURCE: Journal of Medicinal Chemistry (1995), 38(13), 2311-16
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



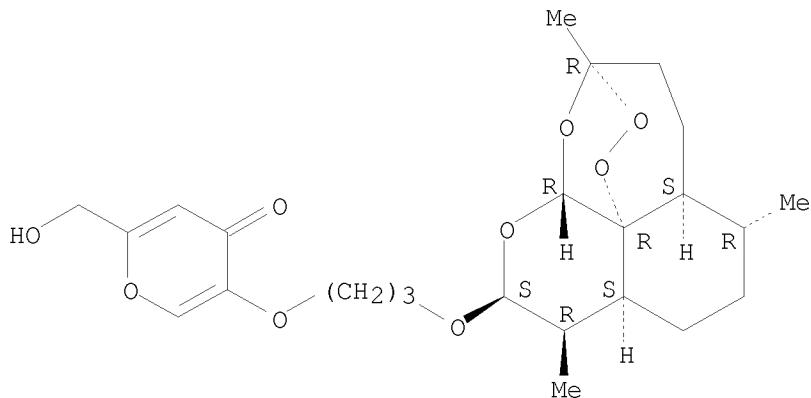
AB Various derivs. of artemisinin covalently linked to iron chelators, e.g. I, were synthesized, and their antimalarial activities were evaluated. Although results show no indication that the presence of an iron chelator in the vicinity of artemisinin potentiates its action, the linked compds. prepared still retain comparable activities to that of artemisinin.

IT 165068-36-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (mechanism-based development of new antimalarials, synthesis of derivs. of artemisinin attached to iron chelators)

RN 165068-36-0 HCPLUS

CN 4H-Pyran-4-one, 3-[3-[(decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyran-4-yl)oxy]propoxy]-6-(hydroxymethyl)-, [3R-(3 α ,5 α β ,6 β ,8 α β ,9 α ,10 α ,12 β ,12aR*)]- (9CI) (CA INDEX NAME)

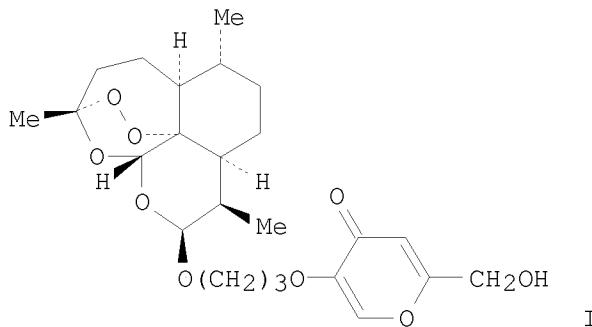
Absolute stereochemistry. Rotation (+).



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L14 ANSWER 1 OF 1 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1995:608133 HCPLUS

DOCUMENT NUMBER: 123:83751
ORIGINAL REFERENCE NO.: 123:15005a, 15008a
TITLE: Mechanism-Based Development of New Antimalarials:
Synthesis of Derivatives of Artemisinin Attached to
Iron Chelators
AUTHOR(S): Kamchonwongpaisan, Sumalee; Paitayatat, Sumpa;
Thebtaranonth, Yodhathai; Wilairat, Prapin; Yuthavong,
Yongyuth
CORPORATE SOURCE: Faculty of Science, Mahidol University, Bangkok,
10400, Thailand
SOURCE: Journal of Medicinal Chemistry (1995),
38(13), 2311-16
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



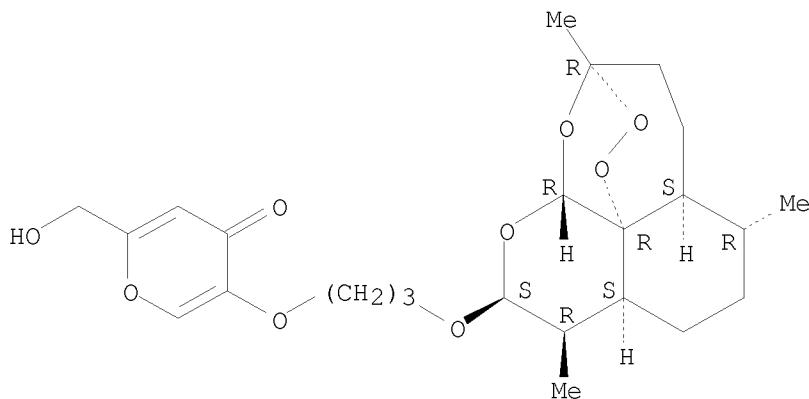
AB Various derivs. of artemisinin covalently linked to iron chelators, e.g. I, were synthesized, and their antimalarial activities were evaluated. Although results show no indication that the presence of an iron chelator in the vicinity of artemisinin potentiates its action, the linked compds. prepared still retain comparable activities to that of artemisinin.

IT 165068-36-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(mechanism-based development of new antimalarials, synthesis of derivs. of artemisinin attached to iron chelators)

RN 165068-36-0 HCAPLUS

CN 4H-Pyran-4-one, 3-[3-[(decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl)oxy]propoxy]-6-(hydroxymethyl)-, [3R-(3 α ,5a β ,6 β ,8a β ,9 α ,10 α ,12 β ,12aR*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



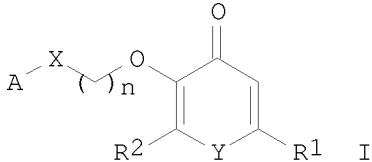
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L17 ANSWER 1 OF 5 HCPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:312673 HCPLUS
DOCUMENT NUMBER: 138:321131
TITLE: Preparation of pyranones for treatment of tumors
related to GTPases.
INVENTOR(S): Leblanc, Veronique; Leblond, Bertrand;
Melle-Milovanovic, Dominique; Lopez Rodriguez, Maria
Luz; Viso Beronda, Alma
PATENT ASSIGNEE(S): Exonhit Therapeutics S.A., Fr.
SOURCE: U.S., 24 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6552073	B1	20030422	US 2002-85141	20020301 <--
CA 2477003	A1	20030912	CA 2003-2477003	20030228 <--
WO 2003074508	A1	20030912	WO 2003-IB1050	20030228 <--
WO 2003074508	B1	20031127		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003209924	A1	20030916	AU 2003-209924	20030228 <--
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

JP 2005529079	T 20050929	JP 2003-572976	20030228
US 20050054629	A1 20050310	US 2004-502625	20041022 <--
PRIORITY APPLN. INFO.:		US 2002-85141	A 20020301
		WO 2003-IB1050	W 20030228

OTHER SOURCE(S): MARPAT 138:321131
GI



AB Title compds. [I; R1 = CH2R3, COR3; R2 = H, alkenyl; R3 = OH, OR4, SR4, NR5R6, pyrrolidinyl, piperidinyl; R4 = alkyl, aryl, aralkyl, alkanoyl, arylcarbonyl; R5, R6 = H, alkyl, aryl, aralkyl; n = 1-10; X = O, S, NR7; Y = O; R7 = H, alkyl, aryl, aralkyl], were prepared. Thus, 5-[7-(3,4-dichloro-2-propylphenoxy)heptyloxy]-2-hydroxymethyl-4H-pyran-4-one (general preparation outlined) showed IC50 = 5-10 μ M against H460 lung carcinoma and HCT116 colon cancer cells, resp.

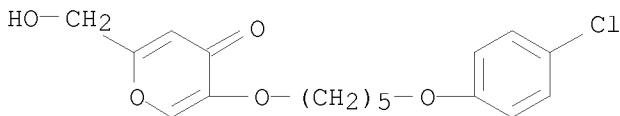
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514170-79-7P 514170-80-0P 514170-81-1P
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514170-85-5P 514170-86-6P 514170-87-7P
514170-88-8P 514170-89-9P 514170-90-2P
514170-91-3P 514170-92-4P 514170-93-5P
514170-94-6P 514170-95-7P 514170-96-8P
514170-97-9P 514170-98-0P 514170-99-1P
514171-00-7P 514171-01-8P 514171-02-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of pyranones for treatment of tumors related to

GTPases)

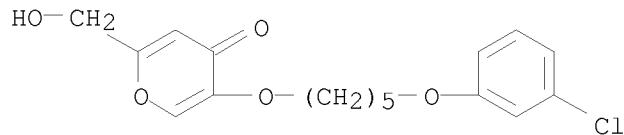
RN 514170-76-4 HCAPLUS

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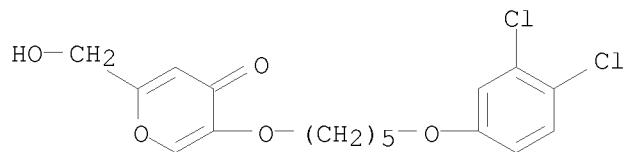


RN 514170-77-5 HCAPLUS

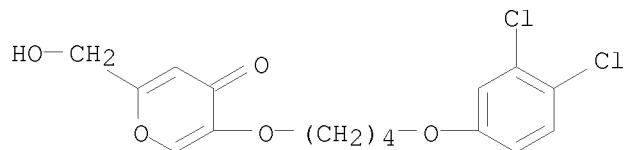
CN 4H-Pyran-4-one, 5-[5-(3-chlorophenoxy)pentyl]oxy]-2-(hydroxymethyl)- (CA INDEX NAME)



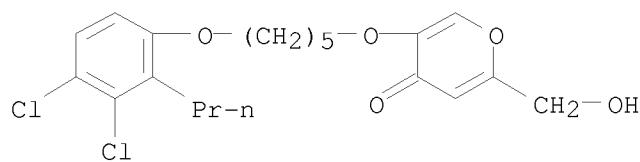
RN 514170-78-6 HCPLUS
 CN 4H-Pyran-4-one, 5-[5-(3,4-dichlorophenoxy)pentyl]oxy]-2-(hydroxymethyl)-
 (CA INDEX NAME)



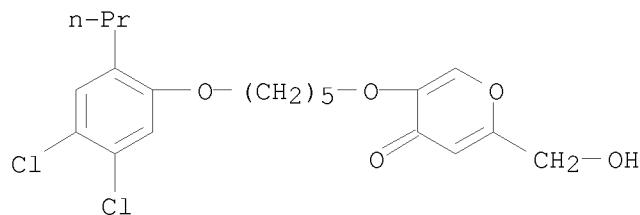
RN 514170-79-7 HCPLUS
 CN 4H-Pyran-4-one, 5-[4-(3,4-dichlorophenoxy)butoxy]-2-(hydroxymethyl)-
 (CA INDEX NAME)



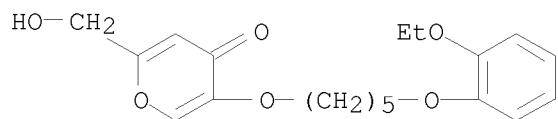
RN 514170-80-0 HCPLUS
 CN 4H-Pyran-4-one, 5-[5-(3,4-dichloro-2-propylphenoxy)pentyl]oxy]-2-(hydroxymethyl)-
 (CA INDEX NAME)



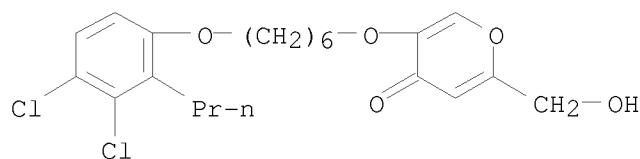
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 CN 4H-Pyran-4-one, 5-[5-(4,5-dichloro-2-propylphenoxy)pentyl]oxy]-2-(hydroxymethyl)-
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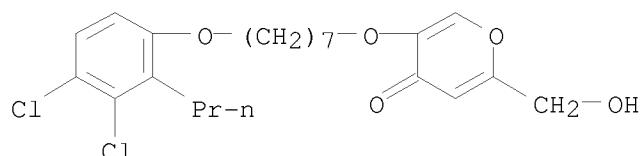
RN 514170-82-2 HCAPLUS
 CN 4H-Pyran-4-one, 5-[5-(2-ethoxyphenoxy)pentyl]oxy]-2-(hydroxymethyl)- (CA INDEX NAME)



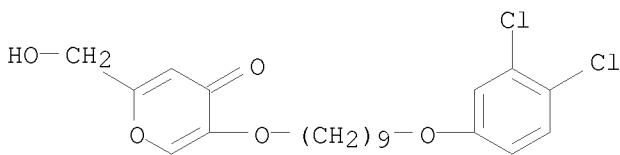
RN 514170-83-3 HCAPLUS
 CN 4H-Pyran-4-one, 5-[6-(3,4-dichloro-2-propylphenoxy)hexyl]oxy]-2-(hydroxymethyl)- (CA INDEX NAME)



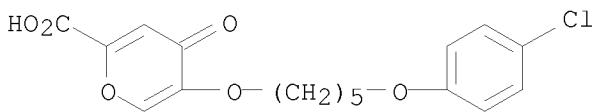
RN 514170-84-4 HCAPLUS
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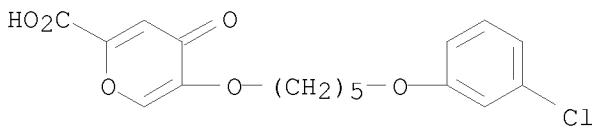
RN 514170-85-5 HCAPLUS
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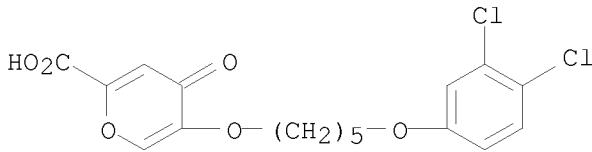
RN 514170-86-6 HCAPLUS
 CN 4H-Pyran-2-carboxylic acid, 5-[5-(4-chlorophenoxy)pentyl]oxy]-4-oxo- (CA INDEX NAME)



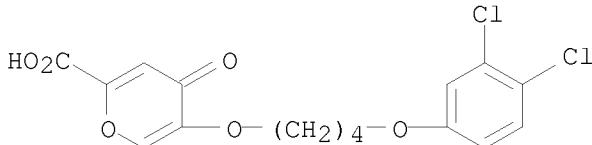
RN 514170-87-7 HCAPLUS
 CN 4H-Pyran-2-carboxylic acid, 5-[5-(3-chlorophenoxy)pentyl]oxy]-4-oxo- (CA INDEX NAME)



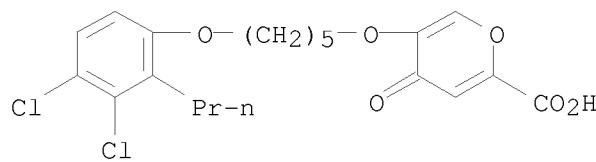
RN 514170-88-8 HCAPLUS
 CN 4H-Pyran-2-carboxylic acid, 5-[5-(3,4-dichlorophenoxy)pentyl]oxy]-4-oxo- (CA INDEX NAME)



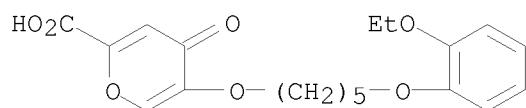
RN 514170-89-9 HCAPLUS
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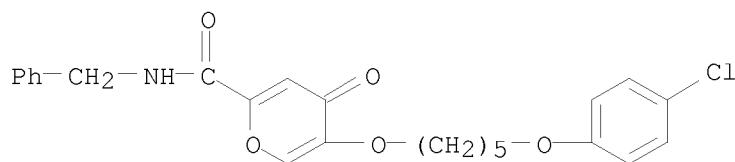
RN 514170-90-2 HCAPLUS
 CN 4H-Pyran-2-carboxylic acid, 5-[5-(3,4-dichloro-2-propylphenoxy)pentyl]oxy]-4-oxo- (CA INDEX NAME)



RN 514170-91-3 HCAPLUS
 CN 4H-Pyran-2-carboxylic acid, 5-[5-(2-ethoxyphenoxy)pentyl]oxy]-4-oxo- (CA INDEX NAME)

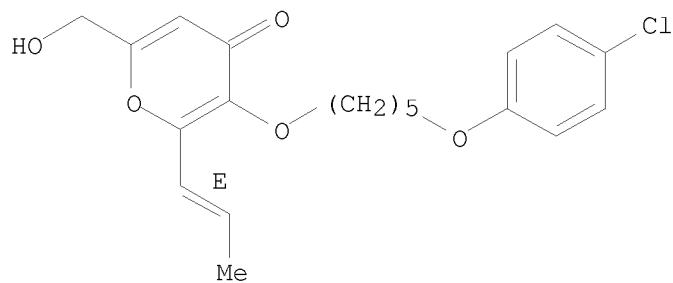


RN 514170-92-4 HCAPLUS
 CN 4H-Pyran-2-carboxamide, 5-[5-(4-chlorophenoxy)pentyl]oxy]-4-oxo-N-(phenylmethyl)- (CA INDEX NAME)



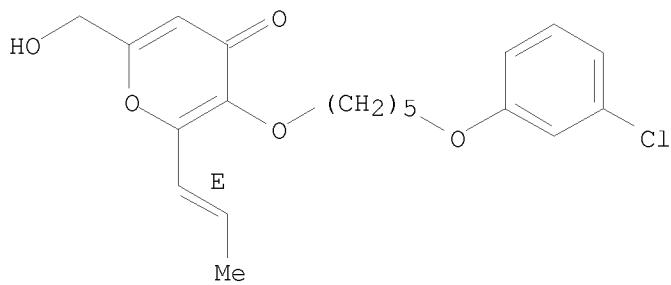
RN 514170-93-5 HCAPLUS
 CN 4H-Pyran-4-one, 3-[5-(4-chlorophenoxy)pentyl]oxy]-6-(hydroxymethyl)-2-(1E)-1-propen-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



RN 514170-94-6 HCAPLUS
 CN 4H-Pyran-4-one, 3-[5-(3-chlorophenoxy)pentyl]oxy]-6-(hydroxymethyl)-2-(1E)-1-propen-1-yl- (CA INDEX NAME)

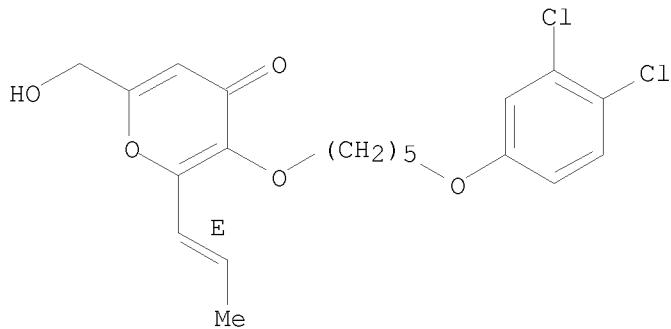
Double bond geometry as shown.



RN 514170-95-7 HCPLUS

CN 4H-Pyran-4-one, 3-[(5-(3,4-dichlorophenoxy)pentyl)oxy]-6-(hydroxymethyl)-2-(1E)-1-propen-1-yl- (CA INDEX NAME)

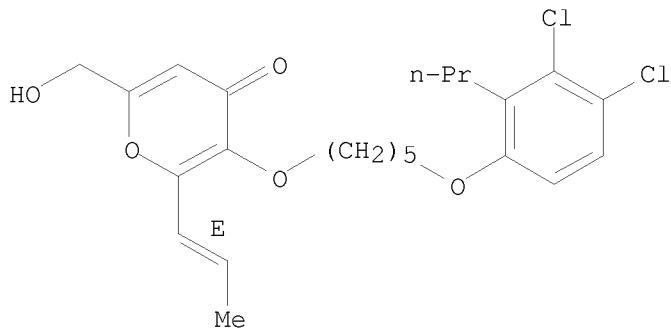
Double bond geometry as shown.



RN 514170-96-8 HCPLUS

CN 4H-Pyran-4-one, 3-[(5-(3,4-dichloro-2-propylphenoxy)pentyl)oxy]-6-(hydroxymethyl)-2-(1E)-1-propen-1-yl- (CA INDEX NAME)

Double bond geometry as shown.

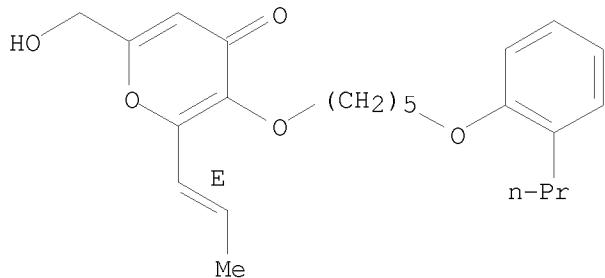


RN 514170-97-9 HCPLUS

CN 4H-Pyran-4-one, 6-(hydroxymethyl)-2-(1E)-1-propen-1-yl-3-[(5-(2-propylphenoxy)pentyl)oxy]- (CA INDEX NAME)

10541328

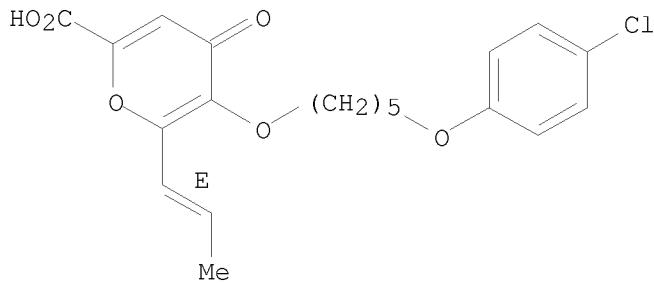
Double bond geometry as shown.



RN 514170-98-0 HCPLUS

CN 4H-Pyran-2-carboxylic acid, 5-[(5-(4-chlorophenoxy)pentyl)oxy]-4-oxo-6-(1E)-1-propen-1-yl- (CA INDEX NAME)

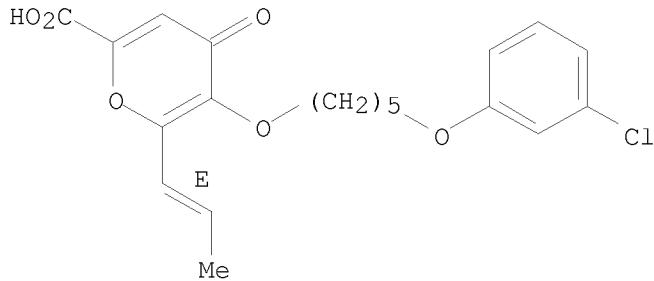
Double bond geometry as shown.



RN 514170-99-1 HCPLUS

CN 4H-Pyran-2-carboxylic acid, 5-[(5-(3-chlorophenoxy)pentyl)oxy]-4-oxo-6-(1E)-1-propen-1-yl- (CA INDEX NAME)

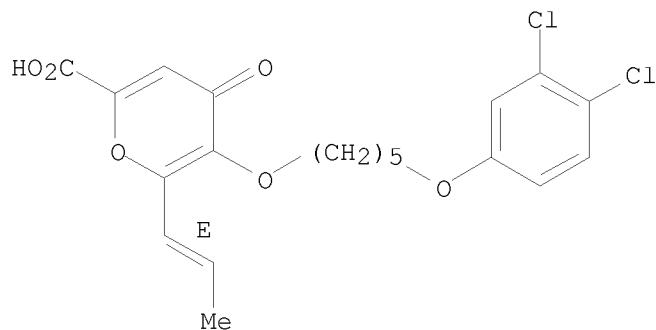
Double bond geometry as shown.



RN 514171-00-7 HCPLUS

CN 4H-Pyran-2-carboxylic acid, 5-[(5-(3,4-dichlorophenoxy)pentyl)oxy]-4-oxo-6-(1E)-1-propen-1-yl- (CA INDEX NAME)

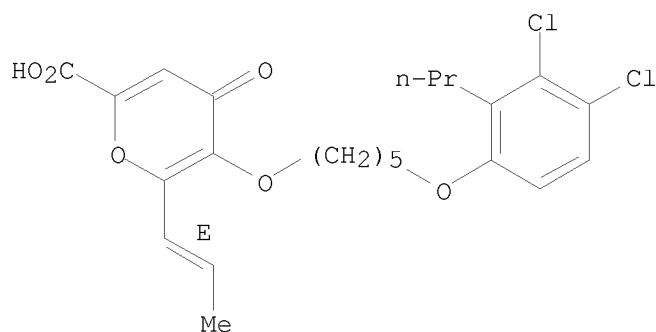
Double bond geometry as shown.



RN 514171-01-8 HCPLUS

CN 4H-Pyran-2-carboxylic acid, 5-[5-(3,4-dichloro-2-propylphenoxy)pentyl]oxy]-4-oxo-6-(1E)-1-propen-1-yl- (CA INDEX NAME)

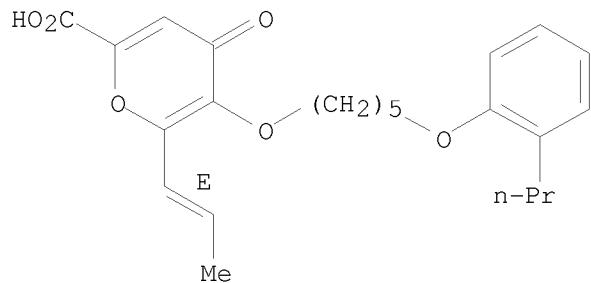
Double bond geometry as shown.



RN 514171-02-9 HCPLUS

CN 4H-Pyran-2-carboxylic acid, 4-oxo-6-(1E)-1-propen-1-yl-5-[5-(2-propylphenoxy)pentyl]oxy- (CA INDEX NAME)

Double bond geometry as shown.

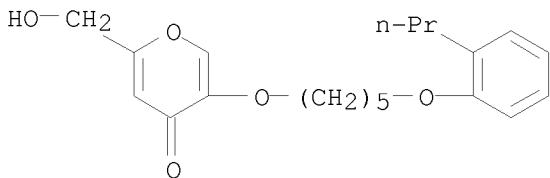


IT 107757-98-2P 107758-01-0P 514171-03-0P

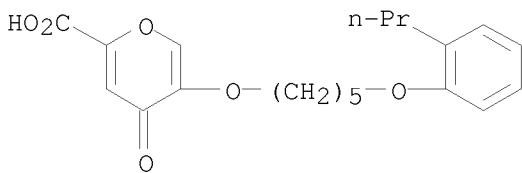
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10541328

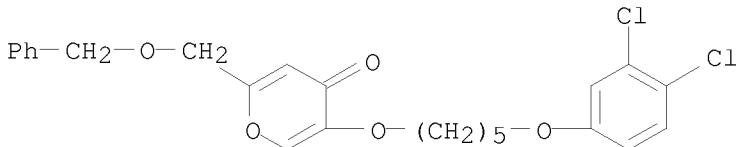
(preparation of pyranones for treatment of tumors related to GTPases)
RN 107757-98-2 HCAPLUS
CN 4H-Pyran-4-one, 2-(hydroxymethyl)-5-[[5-(2-propylphenoxy)pentyl]oxy]- (CA
INDEX NAME)



RN 107758-01-0 HCAPLUS
CN 4H-Pyran-2-carboxylic acid, 4-oxo-5-[[5-(2-propylphenoxy)pentyl]oxy]- (CA
INDEX NAME)



RN 514171-03-0 HCAPLUS
CN 4H-Pyran-4-one, 5-[[5-(3,4-dichlorophenoxy)pentyl]oxy]-2-
[(phenylmethoxy)methyl]- (CA INDEX NAME)

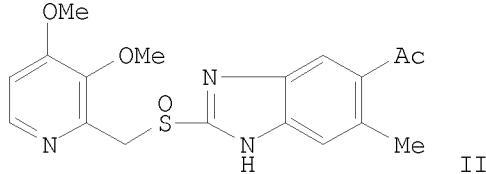
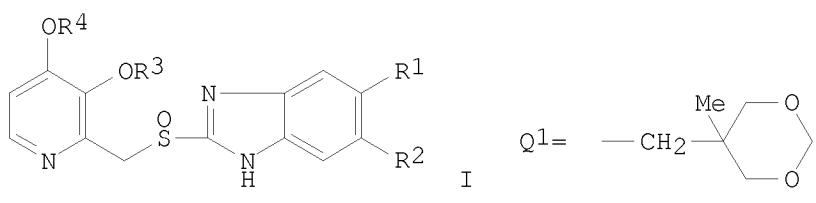


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:151767 HCAPLUS
DOCUMENT NUMBER: 116:151767
ORIGINAL REFERENCE NO.: 116:25692h, 25693a
TITLE: Preparation of (pyridinylmethylsulfinyl)benzimidazoles
as gastric acid secretion inhibitors
INVENTOR(S): Braendstroem, Arne Elof; Lindberg, Per Lennart;
Sunden, Gunnel Elisabeth
PATENT ASSIGNEE(S): Astra AB, Swed.
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9119712	A1	19911226	WO 1991-SE416	19910611 <--
W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, PL, RO, SD, SE, SU				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG				
CA 2083606	A1	19911221	CA 1991-2083606	19910611 <--
CA 2083606	C	20010821		
AU 9180617	A	19920107	AU 1991-80617	19910611 <--
AU 649456	B2	19940526		
HU 62882	A2	19930628	HU 1992-4034	19910611 <--
JP 05507714	T	19931104	JP 1991-511436	19910611 <--
JP 3049367	B2	20000605		
EP 593463	A1	19940427	EP 1991-911618	19910611 <--
EP 593463	B1	19990915		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
PL 165898	B1	19950228	PL 1991-297295	19910611 <--
RO 110497	B1	19960130	RO 1992-1543	19910611 <--
AT 184602	T	19991015	AT 1991-911618	19910611 <--
ES 2140391	T3	20000301	ES 1991-911618	19910611 <--
IL 98472	A	19950831	IL 1991-98472	19910612 <--
CN 1058213	A	19920129	CN 1991-105025	19910620 <--
CZ 279434	B6	19950412	CZ 1991-1893	19910620 <--
US 5430042	A	19950704	US 1991-718188	19910620 <--
NO 9204650	A	19921202	NO 1992-4650	19921202 <--
LV 10269	B	19951020	LV 1993-820	19930630 <--
PRIORITY APPLN. INFO.:			SE 1990-2206	A 19900620
			SE 1990-2207	A 19900620
			WO 1991-SE416	A 19910611

OTHER SOURCE(S): MARPAT 116:151767
GI

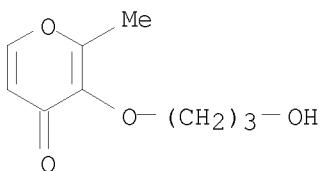


AB Title compds. (I; R1, R2 = H, alkyl, COR5; R3, R4 = Me, Et, cyclopropylmethyl, MeOCH2CH2, Q1; R3R4 = (CH2)n; n = 1-3; R5 = alkyl, alkoxy; one of R1, R2 is always COR5) were prepared. Thus,

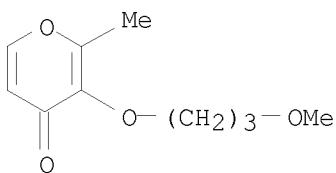
5-acetyl-6-methyl-2-mercaptop-1H-benzimidazole, 3,4-dimethoxy-2-chloromethylpyridine, NaOH, and H₂O were refluxed in EtOH to give 62% coupling product, which was oxidized with 3-C₁C₆H₄C(O)OOH/NaHCO₃ in CH₂C₁₂/H₂O to give title compound II. II inhibited gastric acid secretion in dogs with ED₅₀ = 0.74 μ mol/kg i.v. Tablets were prepared containing II.

IT 139645-13-9P 139645-14-0P 139645-15-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for ulcer inhibitor)

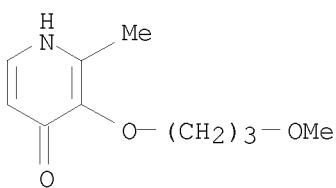
RN 139645-13-9 HCPLUS
 CN 4H-Pyran-4-one, 3-(3-hydroxypropoxy)-2-methyl- (CA INDEX NAME)



RN 139645-14-0 HCPLUS
 CN 4H-Pyran-4-one, 3-(3-methoxypropoxy)-2-methyl- (CA INDEX NAME)



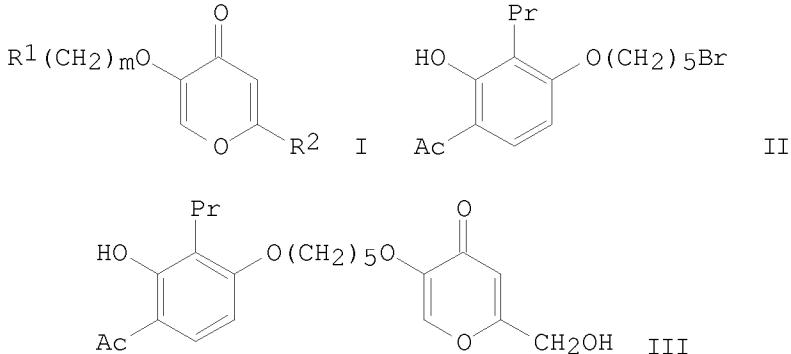
RN 139645-15-1 HCPLUS
 CN 4(1H)-Pyridinone, 3-(3-methoxypropoxy)-2-methyl- (CA INDEX NAME)



L17 ANSWER 3 OF 5 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1987:156276 HCPLUS
 DOCUMENT NUMBER: 106:156276
 ORIGINAL REFERENCE NO.: 106:25429a, 25432a
 TITLE: Preparation of aralkoxy- and aryloxyalkoxy-substituted
 kojic acid derivatives as LTD₄ inhibitors
 INVENTOR(S): Masateru, Miyano; Shone, Robert L.
 PATENT ASSIGNEE(S): G.D. Searle and Co., USA
 SOURCE: U.S., 11 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4644071	A	19870217	US 1984-629916	19840711 <--
US 4705871	A	19871110	US 1986-894591	19860808 <--
US 4812584	A	19890314	US 1987-77362	19870724 <--
PRIORITY APPLN. INFO.:			US 1984-629916	A3 19840711
			US 1986-894591	A3 19860808
OTHER SOURCE(S):		CASREACT 106:156276; MARPAT 106:156276		
GI				



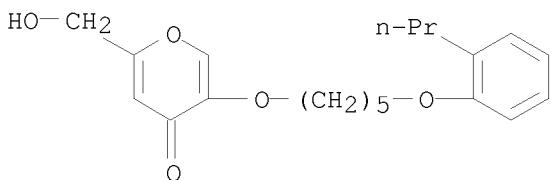
AB Title derivs. I [R1 = naphthyl, naphthoxy, 1,2,3,4-tetrahydronaphth-1- or -2-yl, (un)substituted PhO; R2 = CH2OH, CHO, alkoxycarbonyl, CO2H and its alkali-metal or ammonium salts; m = 1-10] are prepared as LTD4 inhibitors (no data). A mixture of 33.2 mmol (bromopentoxy)acetophenone derivative II (preparation given), 26.6 mmol kojic acid, and 60 mmol anhydrous K2CO3 in DMF was stirred at room temperature for 3 days to give 3.0 g of (phenoxyphenoxy)pyranone derivative III, a preferred compound

IT 107757-98-2P 107757-99-3P 107758-00-9P
 107758-01-0P 107758-02-1P 107758-03-2P
 107758-04-3P 107758-05-4P 107759-81-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as LTD4 inhibitor)

RN 107757-98-2 HCAPLUS

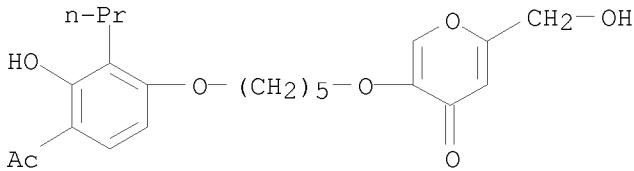
CN 4H-Pyran-4-one, 2-(hydroxymethyl)-5-[[5-(2-propylphenoxy)pentyl]oxy]- (CA INDEX NAME)



10541328

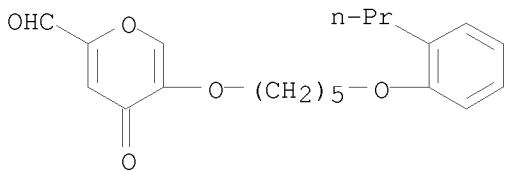
RN 107757-99-3 HCAPLUS

CN 4H-Pyran-4-one, 5-[5-(4-acetyl-3-hydroxy-2-propylphenoxy)pentyl]oxy]-2-(hydroxymethyl)- (CA INDEX NAME)



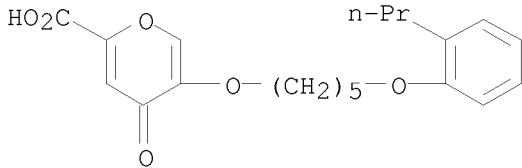
RN 107758-00-9 HCAPLUS

CN 4H-Pyran-2-carboxaldehyde, 4-oxo-5-[5-(2-propylphenoxy)pentyl]oxy]- (CA INDEX NAME)



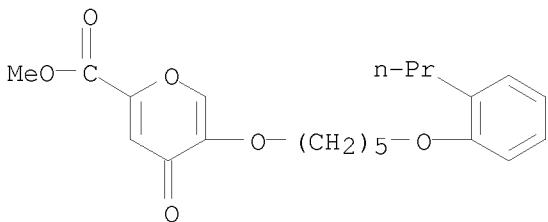
RN 107758-01-0 HCAPLUS

CN 4H-Pyran-2-carboxylic acid, 4-oxo-5-[5-(2-propylphenoxy)pentyl]oxy]- (CA INDEX NAME)



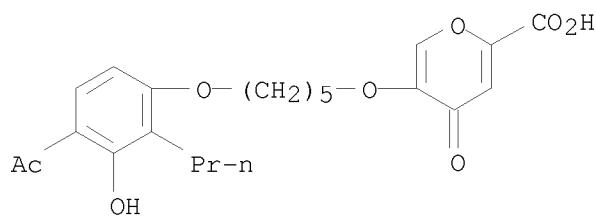
RN 107758-02-1 HCAPLUS

CN 4H-Pyran-2-carboxylic acid, 4-oxo-5-[5-(2-propylphenoxy)pentyl]oxy]-, methyl ester (CA INDEX NAME)



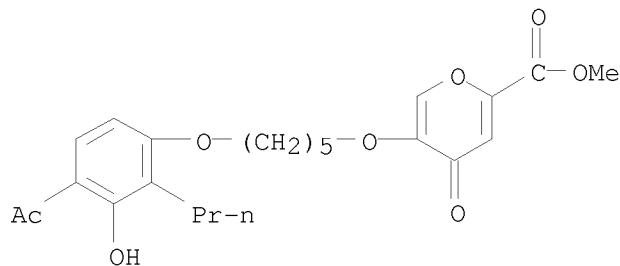
RN 107758-03-2 HCAPLUS

CN 4H-Pyran-2-carboxylic acid, 5-[5-(4-acetyl-3-hydroxy-2-propylphenoxy)pentyl]oxy]-4-oxo- (CA INDEX NAME)



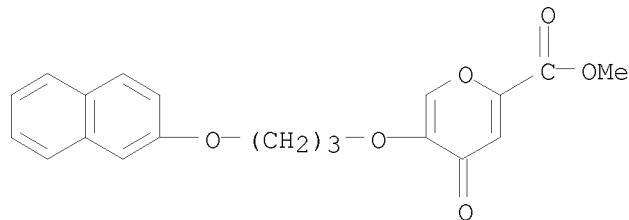
RN 107758-04-3 HCAPLUS

CN 4H-Pyran-2-carboxylic acid, 5-[5-(4-acetyl-3-hydroxy-2-propylphenoxy)pentyl]oxy]-4-oxo-, methyl ester (CA INDEX NAME)



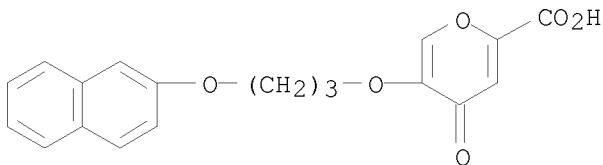
RN 107758-05-4 HCAPLUS

CN 4H-Pyran-2-carboxylic acid, 5-[3-(2-naphthalenyloxy)propoxy]-4-oxo-, methyl ester (CA INDEX NAME)



RN 107759-81-9 HCAPLUS

CN 4H-Pyran-2-carboxylic acid, 5-[3-(2-naphthalenyloxy)propoxy]-4-oxo-, sodium salt (9CI) (CA INDEX NAME)



● Na

L17 ANSWER 4 OF 5 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:515074 HCPLUS

DOCUMENT NUMBER: 105:115074

ORIGINAL REFERENCE NO.: 105:18634h, 18635a

TITLE: Heterocyclic compounds and their use

INVENTOR(S): Kiyoshi, Murase; Toshiyasu, Mase; Hiromu, Hara; Kenichi, Tomioka

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 94 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

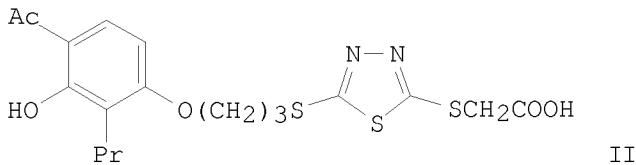
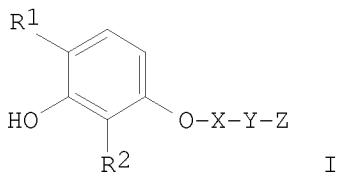
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 181779	A1	19860521	EP 1985-308227	19851112 <--
EP 181779	B1	19940316		
R: AT, BE, CH, ZA 8508493	DE, FR, GB, IT, LI, NL, SE A	19860730	ZA 1985-8493	19851105 <--
ES 548772	A1	19870901	ES 1985-548772	19851111 <--
SU 1470186	A3	19890330	SU 1985-3979033	19851111 <--
JP 62174057	A	19870730	JP 1985-253562	19851112 <--
JP 63035626	B	19880715		
CA 1269982	A1	19900605	CA 1985-495080	19851112 <--
AT 102930	T	19940415	AT 1985-308227	19851112 <--
ES 556746	A1	19871216	ES 1986-556746	19860625 <--
ES 556747	A1	19871216	ES 1986-556747	19860625 <--
ES 556748	A1	19871216	ES 1986-556748	19860625 <--
ES 556749	A1	19871216	ES 1986-556749	19860625 <--
ES 556750	A1	19871216	ES 1986-556750	19860625 <--
ES 556751	A1	19871216	ES 1986-556751	19860625 <--
ES 556752	A1	19871216	ES 1986-556752	19860625 <--
ES 556753	A1	19871216	ES 1986-556753	19860625 <--
SU 1438610	A3	19881115	SU 1986-4028334	19861021 <--
SU 1491337	A3	19890630	SU 1986-4028351	19861024 <--
SU 1498389	A3	19890730	SU 1986-4028367	19861024 <--
SU 1452481	A3	19890115	SU 1986-4028381	19861027 <--
SU 1493105	A3	19890707	SU 1986-4028350	19861027 <--
SU 1454249	A3	19890123	SU 1986-4028405	19861029 <--
US 4855310	A	19890808	US 1988-173734	19880325 <--
US 4908368	A	19900313	US 1989-362959	19890607 <--

US 5177215	A	19930105	US 1990-486550	19900228 <--
US 5258395	A	19931102	US 1992-960125	19921013 <--
PRIORITY APPLN. INFO.:			JP 1984-238991	A 19841112
			JP 1985-219327	A 19851001
			US 1985-796628	A2 19850811
			EP 1985-308227	A 19851112
			US 1988-173734	A3 19880325
			US 1989-362959	A3 19890607
			US 1990-486550	A3 19900228

OTHER SOURCE(S): CASREACT 105:115074; MARPAT 105:115074
GI

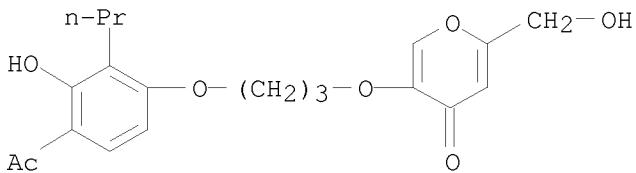


AB Heterocyclic compds. [I; R1 = C1-6 acyl; R2 = C1-6 alkyl; X = C1-6 alkylene or hydroxyalkylene; Y = O, S, carbonylimino, iminocarbonyl; Z = (un)substituted 5- or 6-membered heterocyclic ring containing O, S, N which may be fused with a benzene ring], useful for the treatment and prevention of allergic diseases, are prepared. Thus, thiadiazole II was prepared by reacting 4-(3-bromopropoxy)-2-hydroxy-3-propylacetophenone and [(5-mercaptop-1,3,4-thiadiazol-2-yl)thio]acetic acid. II antagonized the actions of SRS-A in guinea pig ileum and trachea and inhibited SRS-A-mediated anaphylactic asthma in conscious guinea pigs. A tablet was formulated containing II 30, lactose 104, starch 57, hydroxypropyl cellulose 4, Ca CM-cellulose 4, and Mg stearate 1 mg.

IT 104073-60-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiallergic)

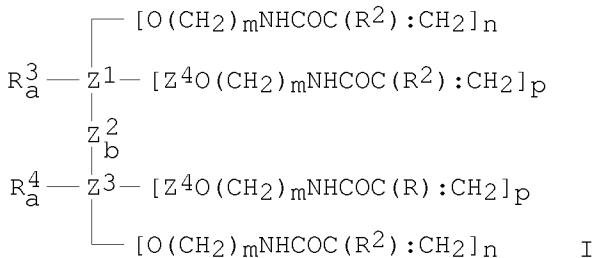
RN 104073-60-1 HCPLUS

CN 4H-Pyran-4-one, 5-[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propoxy]-2-(hydroxymethyl)- (CA INDEX NAME)



L17 ANSWER 5 OF 5 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1986:461480 HCPLUS
 DOCUMENT NUMBER: 105:61480
 ORIGINAL REFERENCE NO.: 105:10055a, 10058a
 TITLE: Unsaturated cyclic amido-substituted ether compounds
 INVENTOR(S): Itoh, Hiroshi; Tanaka, Tomio; Nitta, Atsuhiko; Kamio, Hideo
 PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan
 SOURCE: Eur. Pat. Appl., 78 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

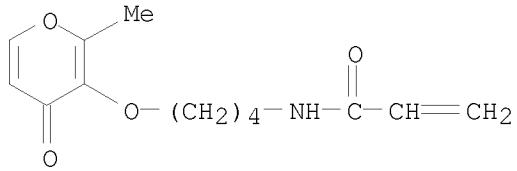
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 155177	A2	19850918	EP 1985-301695	19850312 <--
EP 155177	A3	19870204		
EP 155177	B1	19901031		
R: CH, DE, FR, GB, IT, LI, NL, SE				
JP 60193955	A	19851002	JP 1984-46532	19840313 <--
JP 05073739	B	19931015		
US 4649219	A	19870310	US 1985-708568	19850306 <--
CA 1244012	A1	19881101	CA 1985-475877	19850306 <--
PRIORITY APPLN. INFO.:			JP 1984-46532	A 19840313
OTHER SOURCE(S):	CASREACT 105:61480; MARPAT 105:61480			
GI				



AB Unsatd. cyclic amido-substituted ether compds. I (Z1, Z3 = cyclic group; Z4 = C1-5 alkylene, C2-5 alkenylene, oxyalkylene group, or aminoalkylene group; R3, R4 = halogen, OH, oxo, CN, NO2, SH, S, or a salt thereof, C1-20 alkyl, C2-15 alkenyl, C1-20 haloalkyl, amine group or substituted amine, H, lower alkyl, a carbonyl group, an acid group or salt thereof, or amidopolymethylene group; Z2 = O, carbonyl, thio, sulfonyl, azo, C1-5 alkylene, C2-5 alkenylene; R2 = H or Me; a = 0-5; m = 4-20; n, p = 0-4 and cannot = 0 at the same time, b = 0 or 1) are useful as crosslinking agents or reactive diluents for hygroscopic polymers. Thus, 1.96 g acrylic amide and 4.0 g 2,2-bis(4-bromobutoxyphenyl)propane were dissolved in 20 mL DMF and heated at 0-5° for 6 h in the presence of KOH and phenothiazine to give 3.01 g 2,2-bis[4-(4-acrylamidobutoxy)phenyl]propane II. N-Acryloylpyrrolidine containing 0.2% II was mixed with 1% tert-butyperoxy-2-ethylhexanoate and polymerized at 40° for 50 h to give a hygroscopic flexible block polymer.

10541328

IT 102414-01-7P
RL: PREP (Preparation)
(preparation of, as crosslinking agent for unsatd. polymers)
RN 102414-01-7 HCPLUS
CN 2-Propenamide, N-[4-[(2-methyl-4-oxo-4H-pyran-3-yl)oxy]butyl]- (CA INDEX
NAME)



=> log y
COST IN U.S. DOLLARS

FULL ESTIMATED COST

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	76.16	657.99

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-9.60	-13.60

STN INTERNATIONAL LOGOFF AT 10:50:17 ON 04 AUG 2008